

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1770	((568/648) or (568/650) or (568/651) or (568/652) or (568/653) or (568/658) or (568/717) or (568/772) or (568/799)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/04/29 07:57
L2	1206147	cobalt or nickel or copper	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 07:58
L3	420	l1 and l2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 07:58
L4	7988432	hydrogen\$6 or reduc\$4	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 07:59
L5	399	l3 and l4	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 07:59
L6	61	"3,4,5-trimethoxytoluene"	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:00
L7	3	l5 and l6	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:07
L8	27	l2 and l4 and l6	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:15
L9	314810	l2 same l4	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:16

EAST Search History

L10	300	I1 and I9	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:16
L11	5134600	platinum or rhodium or iron or silver or molybdenum or tungsten or manganese or rhenium or zinc or cadmium or lead or aluminum or zirconium or tin or phosphorus or silicon or arsenic or antimony or bismuth or titanium	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:19
L12	258	I10 and I11	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:19
L13	2862552	oxide or hydroxide or nitrate or chloride or acetate or formate or sulfate	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:20
L14	244	I12 and I13	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:43
L15	212574	aldehyde	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:43
L16	85	I14 and I15	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:43
L17	398497	toluene or toluol	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:44
L18	20	"I116" and I17	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:44

EAST Search History

L19	52	I16 and I17	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:53
L20	34784	bottke.in. or fischer.in. or nobel.in. or rosch.in.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:54
L21	40506	benzaldehyde or benzl near2 alcohol	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:55
L22	39	I17 and I20 and I21	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 08:58
L23	9907	I2 and I4 and I17 and I21	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 09:01
L24	9454	I23 and I11 and I13	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 09:00
L25	288	I2 same I4 same I17 same I21	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 09:01
L26	237	I25 and I11 and I13	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/04/29 09:02

10/500,718

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1204rxw

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS	4	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	5	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	6	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	7	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	8	JAN 30	Saved answer limit increased
NEWS	9	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	10	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	11	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	12	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	13	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS	14	FEB 28	TOXCENTER reloaded with enhancements
NEWS	15	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS	16	MAR 01	INSPEC reloaded and enhanced
NEWS	17	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	18	MAR 08	X.25 communication option no longer available after June 2006
NEWS	19	MAR 22	EMBASE is now updated on a daily basis
NEWS	20	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	21	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	22	APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS	23	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	24	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	25	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS EXPRESS			FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * *

COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

Dear valued STN customer,

In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: <http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW>

Thank you in advance for your participation.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1

DICTIONARY FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\Documents and Settings\rkeys\My Documents\STNEXP4\TEMPLATE\STANDARD\10500718.str

²CH—O

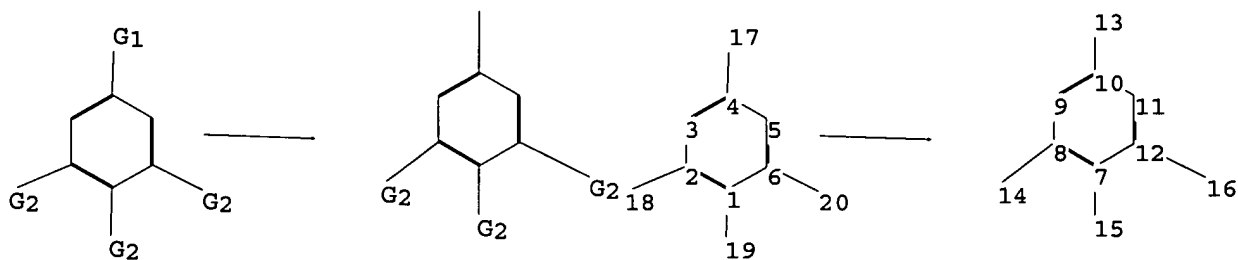
³J—Ak

²₂₄—₂₅

³₂₈—₂₉

₁CH₂—O

₁₂₁—₂₂



chain nodes :

13 14 15 16 17 18 19 20 21 22 24 25 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

1-19 2-18 4-17 6-20 7-15 8-14 10-13 12-16 21-22 24-25 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-19 2-18 4-17 6-20 7-15 8-14 12-16 24-25 28-29

exact bonds :

10-13 21-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:CHO, [*1], [*2]

G2:OH, [*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 29:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

10/500,718

containing 1

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d

L2 HAS NO ANSWERS

L1 STR

29 O M1

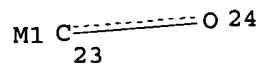
M1

C 27

|||

O

28



2



RRT

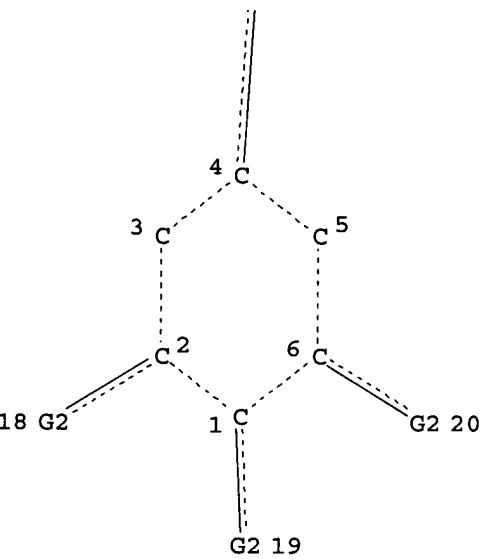
PRO

G1 17
11

5 O-----Ak 26

C 13
|

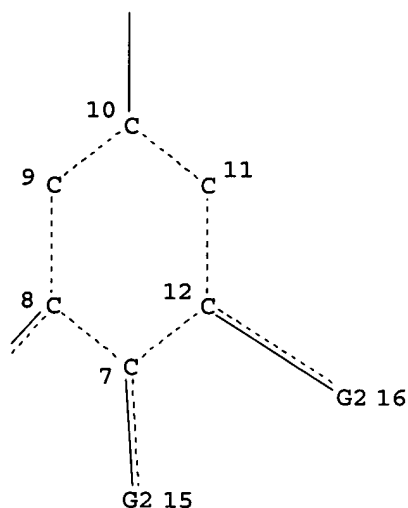
Page 1-B



14 G2

Page 2-A

10/500,718



Page 2-B

VAR G1=27/21/23

VAR G2=29/25

NODE ATTRIBUTES:

HCOUNT	IS	M2	AT	21
HCOUNT	IS	M1	AT	23
HCOUNT	IS	M1	AT	27
HCOUNT	IS	M1	AT	29
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12
NSPEC	IS	C	AT	13
NSPEC	IS	C	AT	14
NSPEC	IS	C	AT	15
NSPEC	IS	C	AT	16
NSPEC	IS	C	AT	17
NSPEC	IS	C	AT	18
NSPEC	IS	C	AT	19
NSPEC	IS	C	AT	20
NSPEC	IS	C	AT	21
NSPEC	IS	C	AT	22
NSPEC	IS	C	AT	23
NSPEC	IS	C	AT	24
NSPEC	IS	C	AT	25
NSPEC	IS	C	AT	26

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 13 21 22 23 24 25 26 27 28 29

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 29

10/500,718

STEREO ATTRIBUTES: NONE
L2 QUE L1

=> file reaction

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.44

0.65

FILE 'CASREACT' ENTERED AT 09:39:12 ON 29 APR 2006
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FILE 'PS' ENTERED AT 09:39:12 ON 29 APR 2006
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=> s 12

SAMPLE SEARCH INITIATED 09:39:24 FILE 'CASREACT'

SCREENING COMPLETE - 25823 REACTIONS TO VERIFY FROM 1479 DOCUMENTS

19.4% DONE 5000 VERIFIED 30 HIT RXNS 12 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 507052 TO 525868
PROJECTED ANSWERS: 1203 TO 2327

SAMPLE SEARCH INITIATED 09:39:26 FILE 'CHEMINFORMRX'
SCREENING COMPLETE - 1516 REACTIONS TO VERIFY FROM 367 DOCUMENTS

66.0% DONE 1000 VERIFIED 23 HIT RXNS 11 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.14

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 28010 TO 32630
PROJECTED ANSWERS: 97 TO 593

2 FILES SEARCHED...

FULL SEARCH INITIATED 09:39:41 FILE 'DJSMONLINE'

SCREENING COMPLETE - 1389 REACTIONS TO VERIFY FROM 1243 DOCUMENTS

73.7% DONE 1023 VERIFIED 10 HIT RXNS 9 DOCS
100.0% DONE 1389 VERIFIED 12 HIT RXNS 11 DOCS
SEARCH TIME: 00.00.34

3 FILES SEARCHED...

FULL SEARCH INITIATED 09:40:17 FILE 'PS'

SCREENING COMPLETE - 223 REACTIONS TO VERIFY FROM 92 DOCUMENTS

100.0% DONE 223 VERIFIED 6 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.04

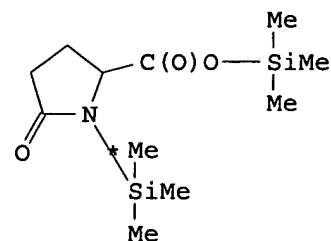
10/500,718

L3 36 L2

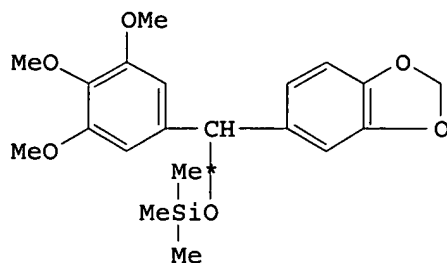
=> d scan

L3 36 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Pyrrolidinones. Synthesis of N-Benzhydrylpyroglutamic Acids and Esters.

RX(7) OF 11 O + P ==> Q...

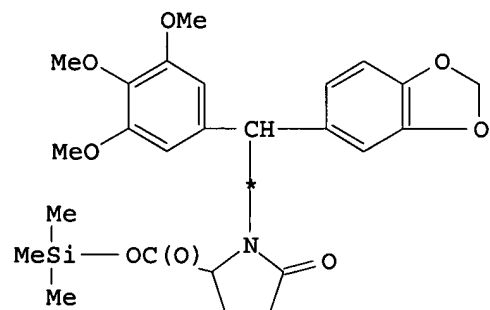


VII



VIII

(7) →



IX

YIELD 94.0%

RX(7) RCT VII, 451110
VIII, 636453
CAT 741 (1493-13-6), CF3-SO3H
PRO IX, 636454
YDS 94.0 %
T 130.0 Cel
KW alkylation; N-alkylation
NTE reaction:VII (VIII) -> IX

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

89.49

90.14

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 21, 2006 (20060421/UP).

10/500,718

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.18

90.32

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1

DICTIONARY FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

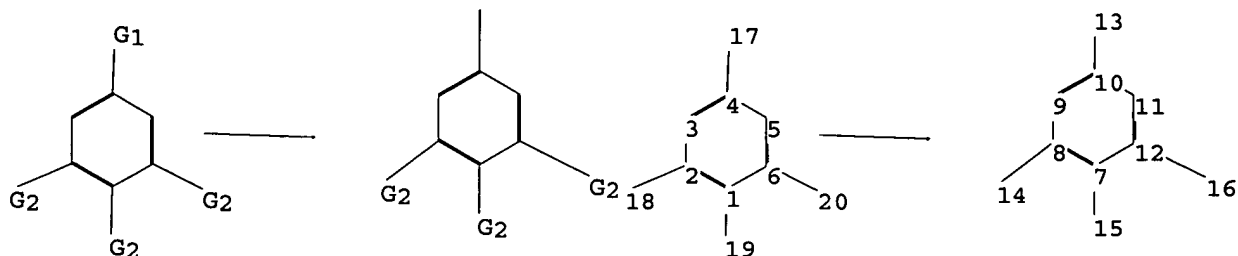
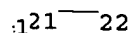
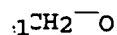
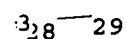
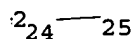
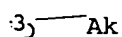
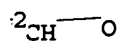
=> screen 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 1839

L4 SCREEN CREATED

=>

Uploading C:\Documents and Settings\rkeys\My Documents\STNEXP4\TEMPLATE\STANDARD\10500718a.str

10/500,718



chain nodes :

13 14 15 16 17 18 19 20 21 22 24 25 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

1-19 2-18 4-17 6-20 7-15 8-14 10-13 12-16 21-22 24-25 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-19 2-18 4-17 6-20 7-15 8-14 12-16 24-25 28-29

exact bonds :

10-13 21-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:CHO, [*1], [*2]

G2:OH, [*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 29:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

containing 1

L5 STRUCTURE UPLOADED

=> que L5 NOT L4

L6 QUE L5 NOT L4

=> file reaction

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

10/500,718

FULL ESTIMATED COST

0.44

90.76

FILE 'CASREACT' ENTERED AT 09:43:37 ON 29 APR 2006
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=> s l6

SAMPLE SEARCH INITIATED 09:43:43 FILE 'CASREACT'
SCREENING COMPLETE - 48 REACTIONS TO VERIFY FROM 31 DOCUMENTS

100.0% DONE 48 VERIFIED 4 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 545 TO 1375
PROJECTED ANSWERS: 3 TO 163

SAMPLE SEARCH INITIATED 09:43:44 FILE 'CHEMINFORMRX'
SCREENING COMPLETE - 15 REACTIONS TO VERIFY FROM 6 DOCUMENTS

100.0% DONE 15 VERIFIED 7 HIT RXNS 4 DOCS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 68 TO 532
PROJECTED ANSWERS: 4 TO 199

FULL SEARCH INITIATED 09:43:49 FILE 'DJSMONLINE'
SCREENING COMPLETE - 25 REACTIONS TO VERIFY FROM 25 DOCUMENTS

100.0% DONE 25 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.07

FULL SEARCH INITIATED 09:43:57 FILE 'PS'
SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L7 8 L6

=> s l6 ful

FULL SEARCH INITIATED 09:44:06 FILE 'CASREACT'
SCREENING COMPLETE - 1028 REACTIONS TO VERIFY FROM 597 DOCUMENTS

100.0% DONE 1028 VERIFIED 84 HIT RXNS 68 DOCS
SEARCH TIME: 00.00.07

FULL SEARCH INITIATED 09:44:14 FILE 'CHEMINFORMRX'
SCREENING
SCREENING
SCREENING COMPLETE - 148 REACTIONS TO VERIFY FROM 100 DOCUMENTS

10/500,718

100.0% DONE 148 VERIFIED 28 HIT RXNS 23 DOCS
SEARCH TIME: 00.00.43

2 FILES SEARCHED...

FULL SEARCH INITIATED 09:44:58 FILE 'DJSMONLINE'
SCREENING COMPLETE - 25 REACTIONS TO VERIFY FROM 25 DOCUMENTS

100.0% DONE 25 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

FULL SEARCH INITIATED 09:45:00 FILE 'PS'
SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

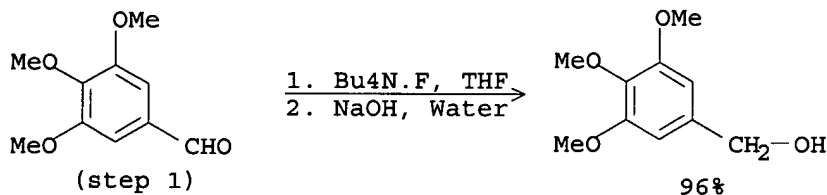
L8 92 L6

=> d scan

L8 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A convenient procedure for the reduction of esters, carboxylic acids, ketones, and aldehydes using tetrabutylammonium fluoride (or Triton B) and polymethylhydrosiloxane

RX(36) OF 43



NOTE: polymethylhydrosiloxane as reagent

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
362.57	453.33

FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 21, 2006 (20060421/UP).

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.18	453.51

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1
DICTIONARY FILE UPDATES: 28 APR 2006 HIGHEST RN 882214-29-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 1839

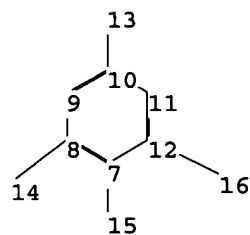
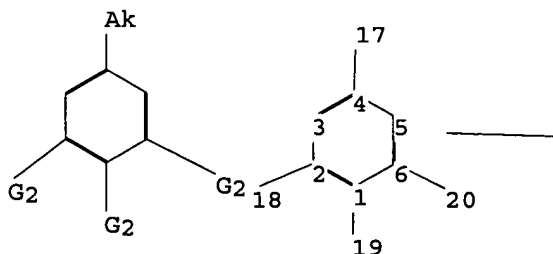
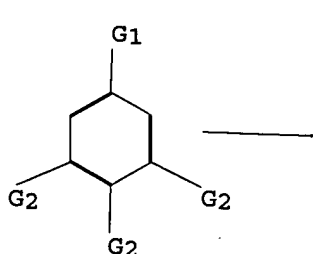
L9 SCREEN CREATED

=>

Uploading C:\Documents and Settings\rkeys\My Documents\STNEXP4\TEMPLATE\STANDARD\10500718b.str

²CH—O ³J—Ak ²₂₄—₂₅ ³₂₈—₂₉

¹CH₂—O ¹₂₁—₂₂



10/500,718

chain nodes :
13 14 15 16 17 18 19 20 21 22 24 25 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-19 2-18 4-17 6-20 7-15 8-14 10-13 12-16 21-22 24-25 28-29
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-19 2-18 4-17 6-20 7-15 8-14 10-13 12-16 24-25 28-29
exact bonds :
21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

G1:CHO, [*1], [*2]

G2:OH, [*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 29:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1

L10 STRUCTURE UPLOADED

=> que L10 NOT L9

L11 QUE L10 NOT L9

=> file reaction
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.44	453.95

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 09:48:18 ON 29 APR 2006
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FILE 'CHEMINFORMRX' ENTERED AT 09:48:18 ON 29 APR 2006
COPYRIGHT (C) FIZ-CHEMIE BERLIN

FILE 'DJSMONLINE' ENTERED AT 09:48:18 ON 29 APR 2006
COPYRIGHT (C) 2006 THE THOMSON CORPORATION

FILE 'PS' ENTERED AT 09:48:18 ON 29 APR 2006
COPYRIGHT (C) 2006 Thieme on STN

=> s l11 sub=18

L8 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see
all L-numbers defined in this session, enter DISPLAY HISTORY at an
arrow prompt (=>). For additional information on subset searching in

10/500,718

this file, enter HELP SUBSET.
ENTER SUBSET L# OR (END):end
SEARCH ENDED BY USER

1 FILES SEARCHED...

L8 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):l6

L6 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):d his

D HIS IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):help subset

Enter the L# of the answer set to be used as a subset. The L# must have been created by a search in this file. To see all L#s created in this session, enter "END" to return to the arrow prompt (=>), followed by "DISPLAY HISTORY". For information about subset searching in this file, enter "HELP SUBSET" at an arrow prompt.

ENTER SUBSET L# OR (END):end

SEARCH ENDED BY USER

2 FILES SEARCHED...

L8 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):(end)

(END) IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):0

0 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):end

SEARCH ENDED BY USER

3 FILES SEARCHED...

L8 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):8

8 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):7

7 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):6

6 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):l6

L6 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):l7

L7 MAY NOT BE USED HERE

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The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

<-----User Break----->

ENTER SUBSET L# OR (END):1

1 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):"end"

"END" IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END):end

SEARCH ENDED BY USER

=> d his

(FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006)

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

L1 STRUCTURE UPLOADED

L2 QUE L1

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:39:12 ON 29 APR 2006

L3 36 S L2

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

L4 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18

L5 STRUCTURE UPLOADED

L6 QUE L5 NOT L4

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:43:37 ON 29 APR 2006

L7 8 S L6

L8 92 S L6

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006

L9 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18

L10 STRUCTURE UPLOADED

L11 QUE L10 NOT L9

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:48:18 ON 29 APR 2006

=> help subset

GENERAL HELP FOR 'SUBSET' IS NOT AVAILABLE

CASREACT

CHEMINFORMRX

DJSMONLINE

PS

ENTER A FILE NAME OR (END):end

=> d his

(FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006)

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

L1 STRUCTURE UPLOADED

10/500,718

L2 QUE L1

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:39:12 ON 29 APR 2006

L3 36 S L2

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

L4 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L5 STRUCTURE UPLOADED
L6 QUE L5 NOT L4

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:43:37 ON 29 APR 2006

L7 8 S L6

L8 92 S L6

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006

L9 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L10 STRUCTURE UPLOADED
L11 QUE L10 NOT L9

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:48:18 ON 29 APR 2006

=> s l11

SAMPLE SEARCH INITIATED 09:56:20 FILE 'CASREACT'

SCREENING COMPLETE - 314 REACTIONS TO VERIFY FROM 151 DOCUMENTS

100.0% DONE 314 VERIFIED 4 HIT RXNS 3 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 5218 TO 7342

PROJECTED ANSWERS: 3 TO 163

SAMPLE SEARCH INITIATED 09:56:22 FILE 'CHEMINFORMRX'

SCREENING COMPLETE - 74 REACTIONS TO VERIFY FROM 48 DOCUMENTS

100.0% DONE 74 VERIFIED 7 HIT RXNS 4 DOCS

SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 965 TO 1995

PROJECTED ANSWERS: 4 TO 199

FULL SEARCH INITIATED 09:56:27 FILE 'DJSMONLINE'

SCREENING COMPLETE - 212 REACTIONS TO VERIFY FROM 206 DOCUMENTS

100.0% DONE 212 VERIFIED 1 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.03

FULL SEARCH INITIATED 09:56:32 FILE 'PS'

SCREENING COMPLETE - 22 REACTIONS TO VERIFY FROM 20 DOCUMENTS

100.0% DONE 22 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

10/500,718

L12 8 L11

=> s l11 ful

FULL SEARCH INITIATED 09:56:42 FILE 'CASREACT'

SCREENING COMPLETE - 5840 REACTIONS TO VERIFY FROM 2782 DOCUMENTS

100.0% DONE 5840 VERIFIED 84 HIT RXNS 68 DOCS

SEARCH TIME: 00.00.08

FULL SEARCH INITIATED 09:56:51 FILE 'CHEMINFORMRX'

SCREENING

SCREENING

SCREENING COMPLETE - 1383 REACTIONS TO VERIFY FROM 899 DOCUMENTS

100.0% DONE 1383 VERIFIED 28 HIT RXNS 23 DOCS

SEARCH TIME: 00.00.46

2 FILES SEARCHED...

FULL SEARCH INITIATED 09:57:38 FILE 'DJSMONLINE'

SCREENING COMPLETE - 212 REACTIONS TO VERIFY FROM 206 DOCUMENTS

100.0% DONE 212 VERIFIED 1 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.08

FULL SEARCH INITIATED 09:57:47 FILE 'PS'

SCREENING COMPLETE - 22 REACTIONS TO VERIFY FROM 20 DOCUMENTS

100.0% DONE 22 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.02

L13 92 L11

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

369.73	823.68
--------	--------

FILE 'STNGUIDE' ENTERED AT 09:59:16 ON 29 APR 2006

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 21, 2006 (20060421/UP).

=> d his

(FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006)

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

L1 STRUCTURE UPLOADED

L2 QUE L1

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:39:12 ON 29 APR 2006

L3 36 S L2

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

L4 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18

L5 STRUCTURE UPLOADED

L6 QUE L5 NOT L4

10/500,718

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:43:37 ON 29 APR 2006

L7 8 S L6
L8 92 S L6

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006

L9 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L10 STRUCTURE UPLOADED
L11 QUE L10 NOT L9

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:48:18 ON 29 APR 2006

L12 8 S L11
L13 92 S L11

FILE 'STNGUIDE' ENTERED AT 09:59:16 ON 29 APR 2006

=> file reaction

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.06	823.74

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 09:59:56 ON 29 APR 2006
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FILE 'CHEMINFORMRX' ENTERED AT 09:59:56 ON 29 APR 2006
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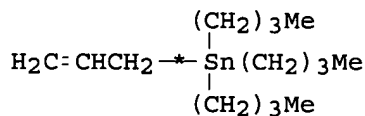
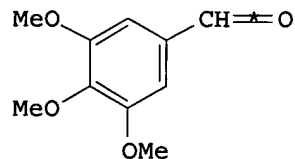
FILE 'DJSMONLINE' ENTERED AT 09:59:56 ON 29 APR 2006
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FILE 'PS' ENTERED AT 09:59:56 ON 29 APR 2006
COPYRIGHT (C) 2006 Thieme on STN

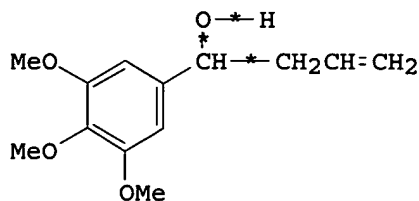
=> d scan l13

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Lanthanum Triflate Catalyzed Allylation of Aldehydes: Crucial Activation
by Benzoic Acid.

RX(7) OF 7 Q + B ==> R



10/500,718



III

YIELD 88.0%

RX(7) RCT I, 43670 (86-81-7)
II, 1987 (24850-33-7;105494-65-3;66680-84-0;66680-85-1)
RGT 475 (65-85-0), Ph-COOH
SOL 6 (75-05-8), MeCN
CAT 393196, La(OTf)₃
PRO III, 868577
YDS 88.0 %
T 25.0 Cel
KW addition; alkylation; C-alkylation
NTE reaction:I (II) -> III, example: 7

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

2.67

826.41

FILE 'STNGUIDE' ENTERED AT 10:00:28 ON 29 APR 2006

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 21, 2006 (20060421/UP).

=> file reaction

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

0.12

826.53

FILE 'CASREACT' ENTERED AT 10:01:51 ON 29 APR 2006

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COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CHEMINFORMRX' ENTERED AT 10:01:51 ON 29 APR 2006

COPYRIGHT (C) FIZ-CHEMIE BERLIN

FILE 'DJSMONLINE' ENTERED AT 10:01:51 ON 29 APR 2006

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FILE 'PS' ENTERED AT 10:01:51 ON 29 APR 2006

COPYRIGHT (C) 2006 Thieme on STN

=> d his

(FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006)

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

L1 STRUCTURE UPLOADED

10/500,718

L2 QUE L1

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:39:12 ON 29 APR 2006

L3 36 S L2

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

L4 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L5 STRUCTURE UPLOADED
L6 QUE L5 NOT L4

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:43:37 ON 29 APR 2006

L7 8 S L6

L8 92 S L6

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006

L9 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L10 STRUCTURE UPLOADED
L11 QUE L10 NOT L9

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:48:18 ON 29 APR 2006

L12 8 S L11

L13 92 S L11

FILE 'STNGUIDE' ENTERED AT 09:59:16 ON 29 APR 2006

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:59:56 ON 29 APR 2006

FILE 'STNGUIDE' ENTERED AT 10:00:28 ON 29 APR 2006

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 10:01:51 ON 29 APR 2006

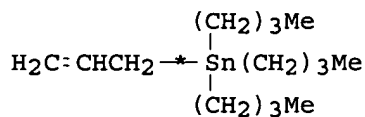
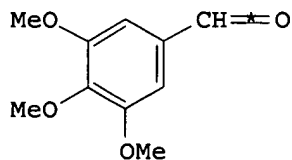
=> d scan l13 2-92

DISPLAY FORMATS NOT ALLOWED WITH SCAN IN A MULTIFILE ENVIRONMENT

=> d scan l13

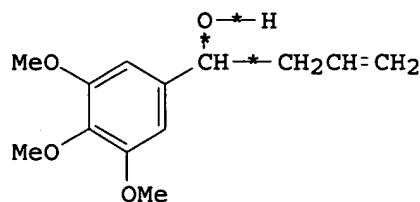
L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Highly Efficient Allylation of Aldehydes and Three-Component Synthesis of Homoallylamines Using Bismuth Triflate Catalyst.

RX(4) OF 9 K + B ==> L



(4) →

10/500,718



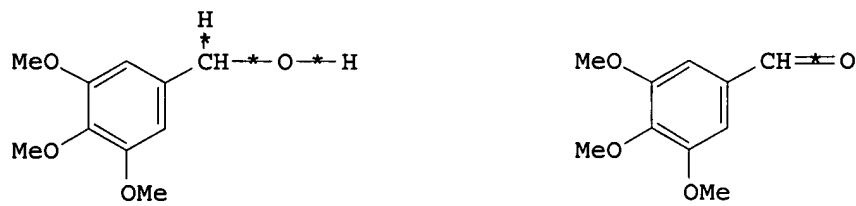
III
YIELD 95.0%

RX(4) RCT I, 43670 (86-81-7)
II, 1987 (24850-33-7;105494-65-3;66680-84-0;66680-85-1)
RGT 475 (65-85-0), Ph-COOH
SOL 6 (75-05-8), MeCN
CAT 561245, Bi(OTf)₃
PRO III, 868577
YDS 95.0 %
T 25.0 Cel
TIM 0.0 hr
KW addition; alkylation; C-alkylation
NTE reaction:I (II) -> III, example: 4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):91

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI A Heterobimetallic Rhodium(I)-Ruthenium(II) Catalyst for the Oppenauer-Type Oxidation of Primary and Secondary Alcohols under Mild Conditions.

RX(8) OF 10 T ==> U



III

IV

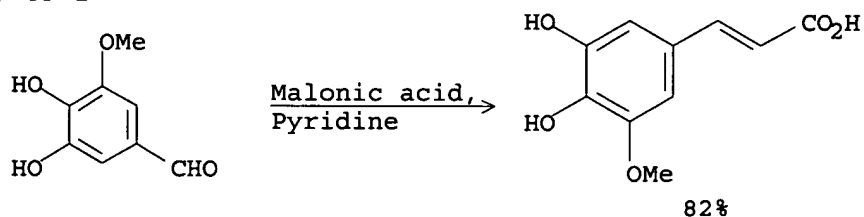
RX(8) RCT III, 203015 (3840-31-1)
RGT 768 (584-08-7), K₂CO₃
SOL 5 (67-64-1), acetone
14 (71-43-2), benzene
CAT 1042988, Ru₂Cl₄(acetone)(PPh₃)₄
1042989, Rh₂Cl₂(C₅Ph₄O)₂
PRO IV, 43670 (86-81-7)
T 25.0 Cel
TIM 24 hr
KW dehydrogenation
NTE reaction:III -> IV, example: 3

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI o-Quinones. XXV. Preparation and properties of o-quinones with electrophilic substituents

10/500,718

RX(1) OF 1

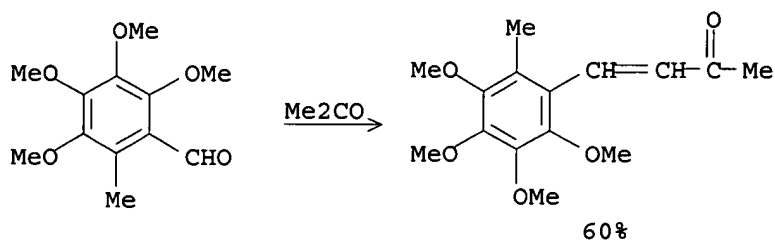


NOTE: Classification: Condensation; Olefination; Decarboxylation; #
Conditions: pyridine piperidine; 20 deg 10 days; 50 deg 10h

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Benzoquinone derivatives

RX(36) OF 74



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Oxidation of benzaldehydes to benzoic acid derivatives by three
Desulfovibrio strains

RX(10) OF 20

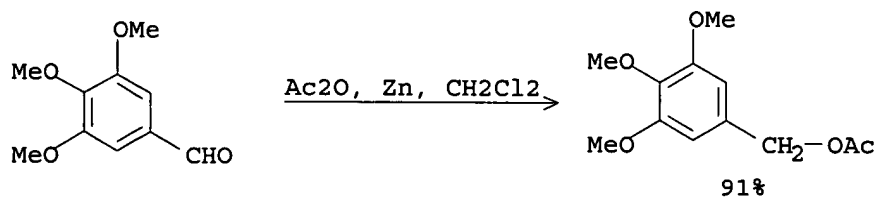


NOTE: Biotransformation: catalyzed by desulfovibrio vulgaris =
desulfovibrio sp.; # Conditions: in nitrogen/carbon dioxide-gas
atmosphere

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A facile one-step conversion of aromatic aldehydes to acetates

RX(4) OF 11



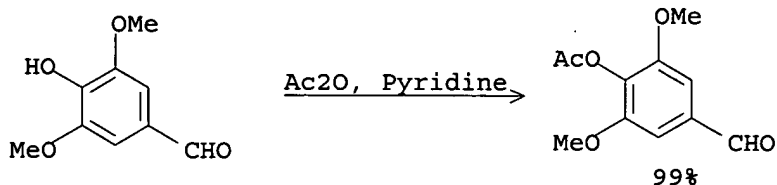
NOTE: acidic alumina catalyst

10/500,718

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Avenanthramides in Oats (*Avena sativa* L.) and Structure-Antioxidant Activity Relationships

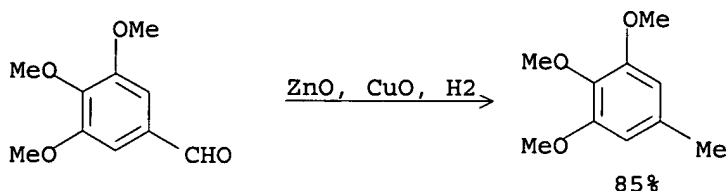
RX(3) OF 11



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Process for producing methyl-substituted aromatic compound

RX(5) OF 10

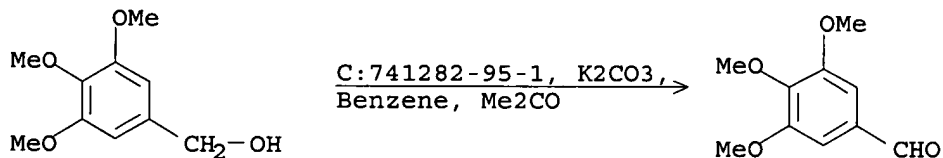


NOTE: thermal

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A Heterobimetallic Rhodium(I)-Ruthenium(II) Catalyst for the Oppenauer-Type Oxidation of Primary and Secondary Alcohols under Mild Conditions

RX(16) OF 19



NOTE: 80% conversion

L13 92 ANSWERS DJSMONLINE COPYRIGHT 2006 THE THOMSON CORP on STN

AN 2003:3299 DJSMONLINE

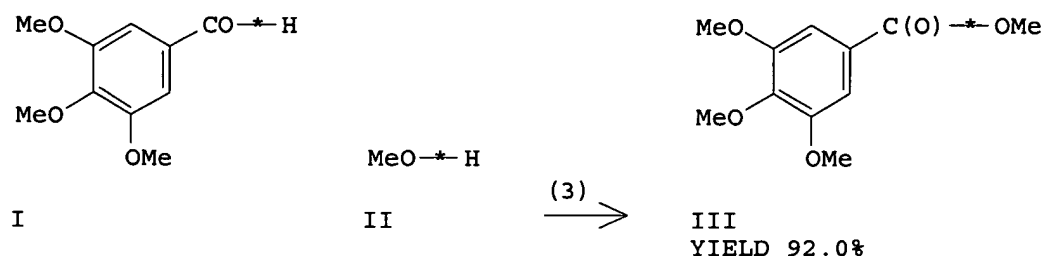
TI CARBOXYLIC ACIDS FROM PRIM . ALCOHOLS ALSO KETONES FROM SEC . ALCOHOLS

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Titanosilicate (TS-1) Catalyzed Oxidation of Aromatic Aldehydes to Esters.

RX(3) OF 5 H + B ==> I

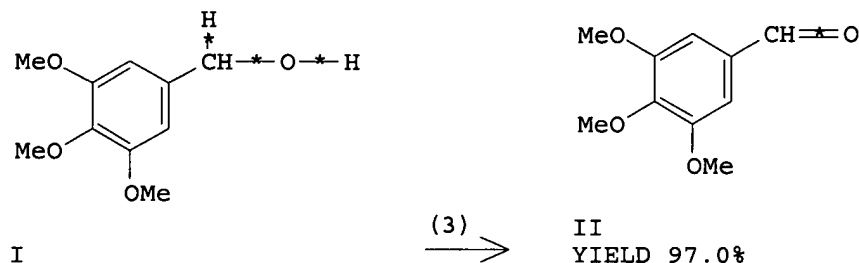
10/500,718



RX(3) RCT I, 43670 (86-81-7)
 II, 123 (67-56-1)
 RGT 1158 (7722-84-1), H2O2
 CAT 5175, Ti-silicalite
 PRO III, 477444
 YDS 92.0 %
 T.KW REFLUX
 TIM 12 hr
 KW acylation; O-acylation; esterification
 NTE reaction:I (II) -> III, example: 3

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
 TI Polyaniline-Supported Vanadium Catalyzed Aerobic Oxidation of Alcohols to Aldehydes and Ketones.

RX(3) OF 11 H ==> I

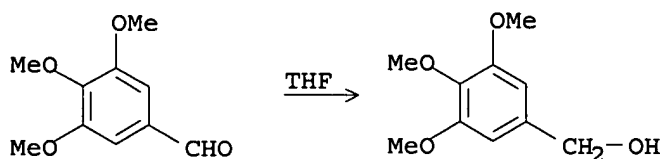


RX(3) RCT I, 203015 (3840-31-1)
 RGT 157 (7782-44-7), O2
 SOL 214 (108-88-3), toluene
 CAT 1023181, VO(acac)2(polyaniline)
 PRO II, 43670 (86-81-7)
 YDS 97.0 %
 T 100.0 Cel
 KW dehydrogenation
 NTE reaction:I -> II, example: 3

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Central stimulants-chemistry and structure activity relations of aralkyl hydrazines

RX(2) OF 11

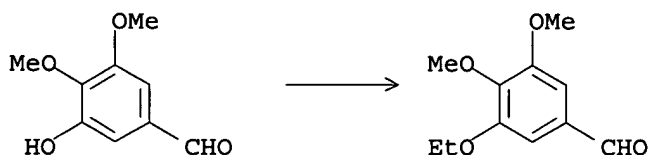


NOTE: Classification: Reduction; # Conditions: LiAlH4 THF Rf 5h

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI The synthesis of hydroxybenzaldehydes from bromobenzaldehydes via lithiated Schiff's bases. Preparation of 5-hydroxypiperonal and related compounds

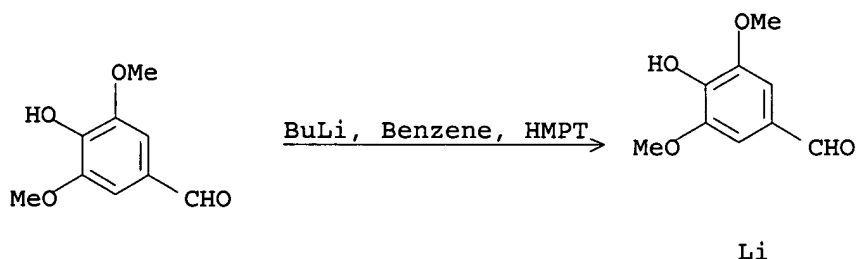
RX(5) OF 6



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Lignans. 10. Preparation of (R)-(+)- and (S)-(-)- β -piperonyl- and - β -veratryl- γ -butyrolactones and their use in the total synthesis of optically active lignans

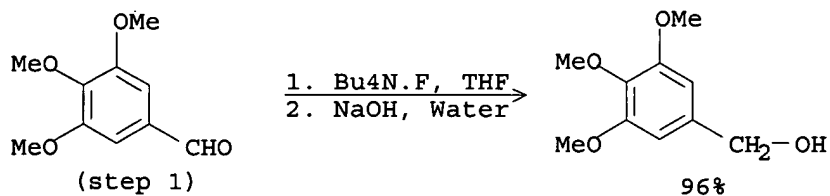
RX(10) OF 77



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A convenient procedure for the reduction of esters, carboxylic acids, ketones, and aldehydes using tetrabutylammonium fluoride (or Triton B) and polymethylhydrosiloxane

RX(36) OF 43



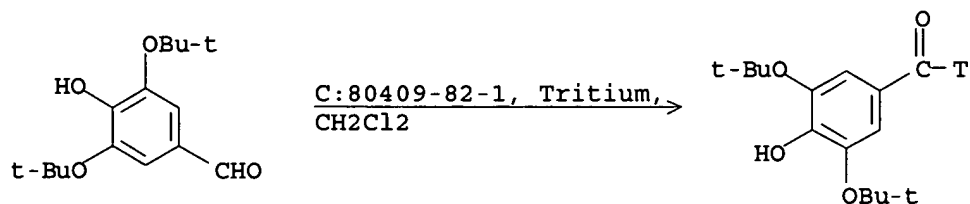
NOTE: polymethylhydrosiloxane as reagent

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Tritium labeling of the PXR ligand GW5801 - an unexpected tritium exchange reaction

10/500,718

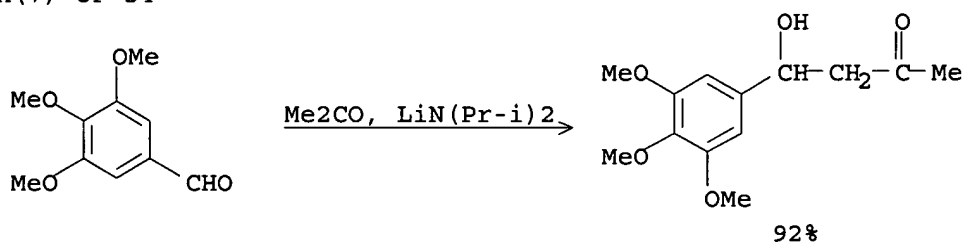
RX(1) OF 5



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Preparation of layered double hydroxides exchanged with diisopropylamide for C-C bond forming reactions

RX(7) OF 54

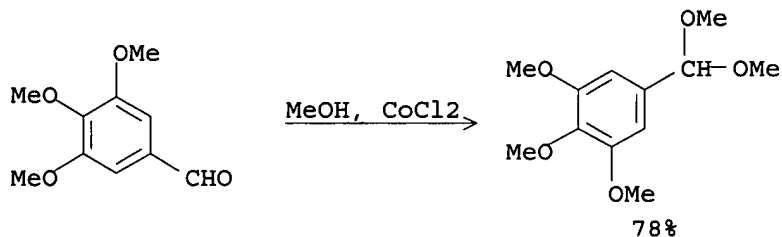


NOTE: solid supported catalyst, Aldol reaction

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Cobalt(II)-catalyzed chemoselective synthesis of acetals from aldehydes

RX(11) OF 20



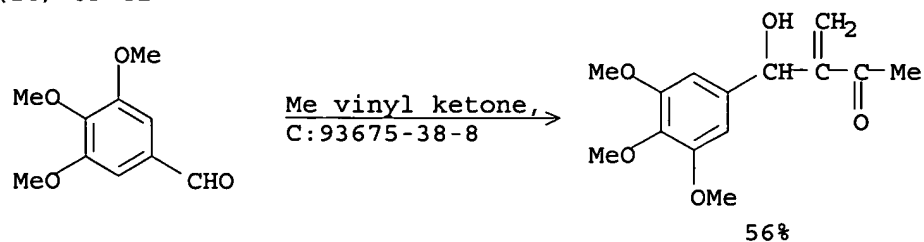
NOTE: chemoselective, green chem.

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI 1-Methylimidazole 3-N-oxide as a new promoter for the Morita-Baylis-Hillman reaction

10/500,718

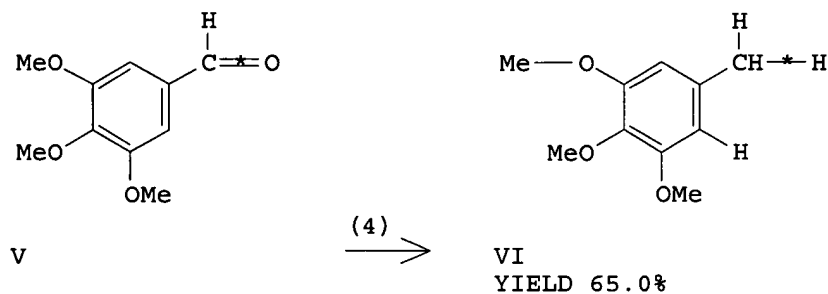
RX(14) OF 41



NOTE: chemoselective, no solvent

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Synthesis of 2,3-Dimethoxy-5-methyl-1,4-benzoquinone: A Key Fragment in Coenzyme-Q Series.

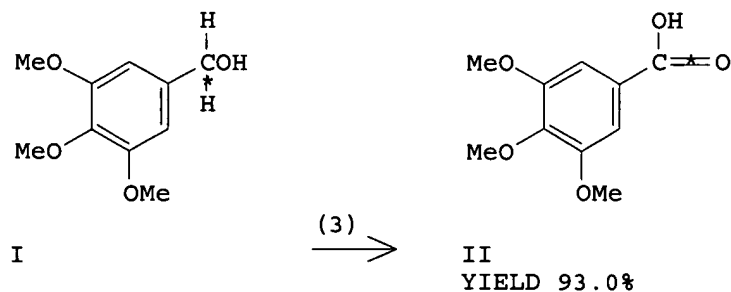
RX(4) OF 15 ...J ==> O...



RX(4) RCT V, 43670 (86-81-7)
RGT 1305 (12714-27-1;11146-96-6), Zn-Hg
SOL 3 (64-19-7), AcOH
222 (7732-18-5), H2O
214 (108-88-3), toluene
PRO VI, 21929 (6443-69-2)
YDS 65.0 %
T.KW REFLUX
NTE reaction:V -> VI

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Copper(II)-Catalyzed Oxidation of Alcohols to Carbonyl Compounds with Hydrogen Peroxide.

RX(3) OF 8 H ==> I



RX(3) RCT I, 203015 (3840-31-1)
RGT 1158 (7722-84-1), H2O2
SOL 6 (75-05-8), MeCN

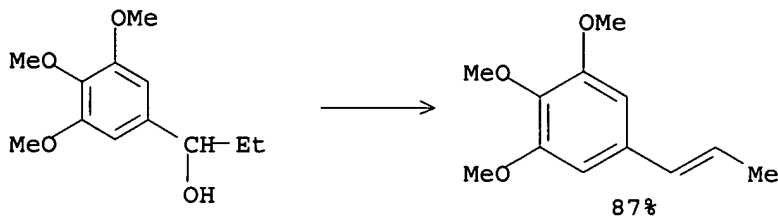
10/500,718

CAT 990542, Cu(H4-salen)
PRO II, 14547 (118-41-2)
YDS 93.0 %
T 80.0 Cel
NTE reaction: I -> II, example: 3

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Colchicine and related compounds. X

RX(1) OF 1

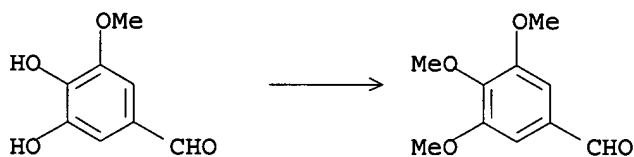


NOTE: Classification: Elimination; Dehydration; # Conditions: I2; vac distil

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI 3,4,5-Trimethoxybenzaldehyde

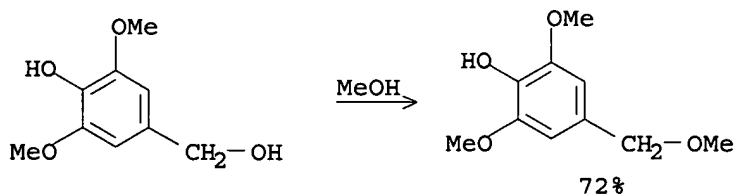
RX(1) OF 1



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Metalation of phenols. Synthesis of benzoquinones by the oxidative degradation approach

RX(5) OF 111

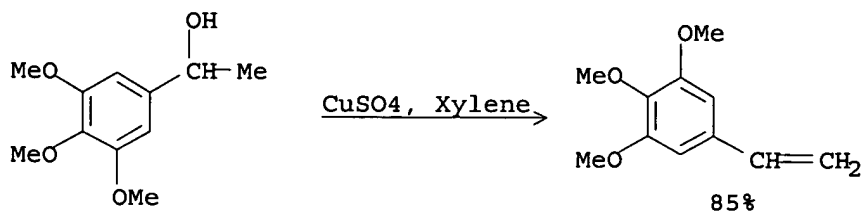


L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Process for preparing methoxy derivatives of styrene

10/500,718

RX(1) OF 3

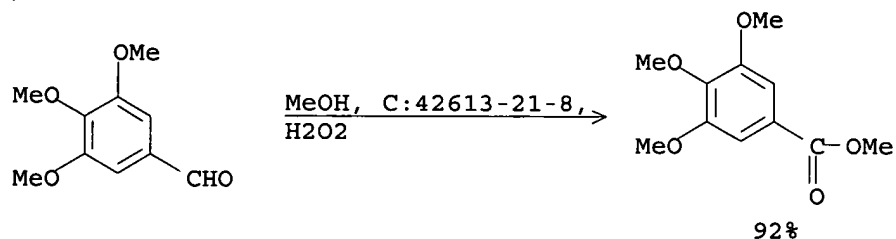


NOTE: reflux, removal of H_2O , 3 h

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Titanosilicate (TS-1) catalyzed oxidation of aromatic aldehydes to esters

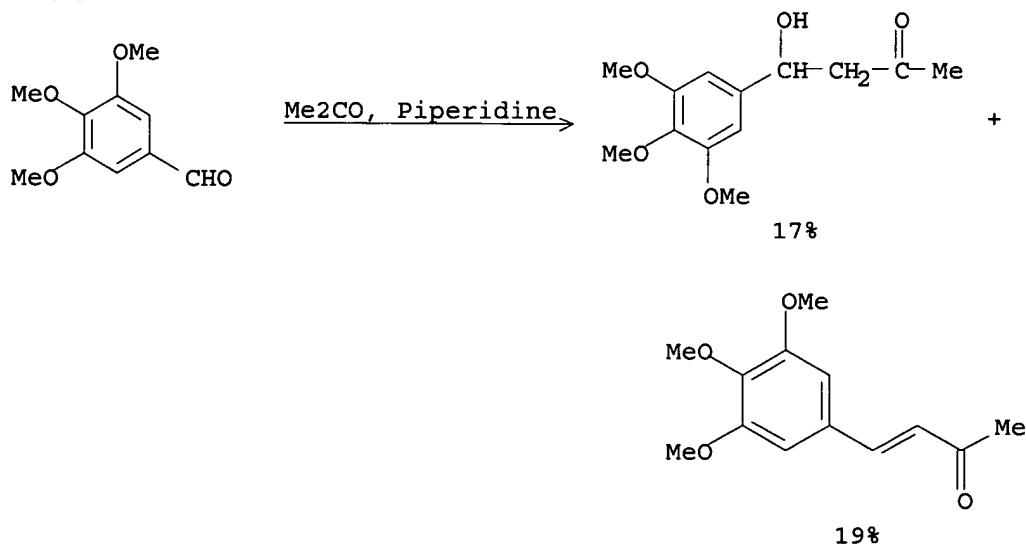
RX(3) OF 4



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Enhanced effect of mesoporous silica on base-catalyzed aldol reaction

RX(4) OF 5



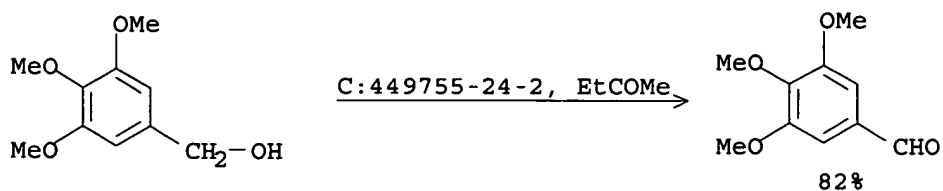
NOTE: FSM-16 was present, Aldol reaction

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Iridium-catalyzed Oppenauer oxidations of benzyl alcohols

10/500,718

RX(12) OF 18

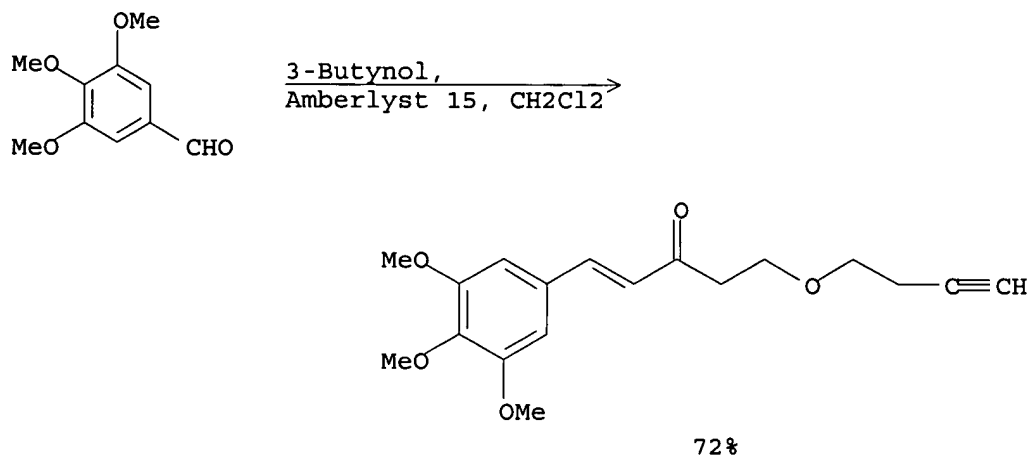


NOTE: Oppenauer oxidn.

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Amberlyst-15 as a novel and recyclable solid acid for the coupling of aromatic aldehydes with homopropargyl alcohol

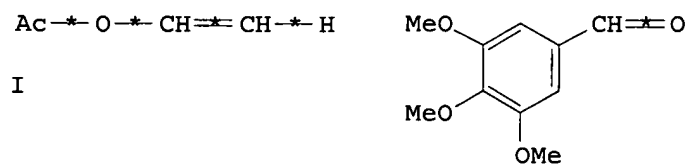
RX(11) OF 13



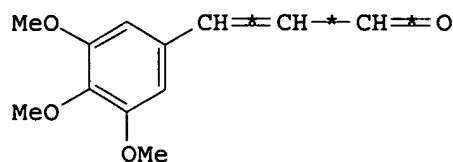
L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Formation of Acetaldehyde Enolate from Vinyl Acetate and Its Reaction with Aromatic and Heterocyclic Aldehydes: An Efficient Synthesis of Enals and Polyenals.

RX(3) OF 11 A + H ==> I



10/500,718



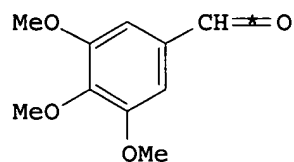
III

YIELD 70.0%

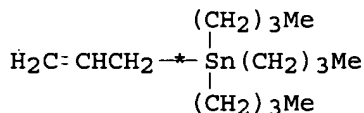
RX(3) RCT I, 2703 (108-05-4)
II, 43670 (86-81-7)
RGT 283 (17194-00-2), Ba(OH)₂
SOL 206 (109-99-9), THF
PRO III, 295885 (34346-90-2;71277-12-8;71277-13-9)
YDS 70.0 %
T.KW REFLUX
NTE reaction:I (II) -> III, example: 3

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Ceric(IV) Ammonium Nitrate: A Novel Reagent for the Synthesis of Homoallyl Alcohols.

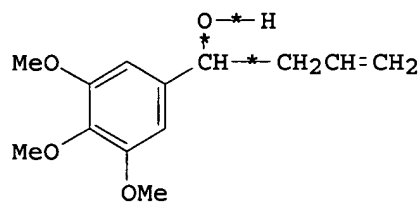
RX(7) OF 14 P + B ==> Q



I



II



III

YIELD 90.0%

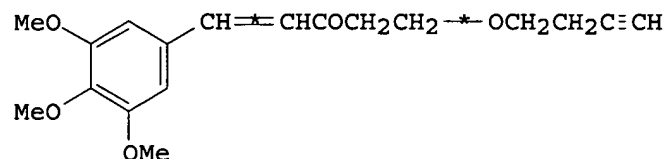
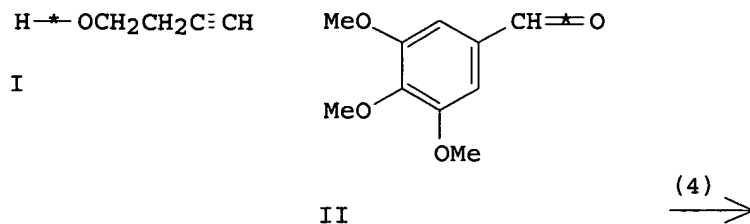
RX(7) RCT I, 43670 (86-81-7)
II, 1987 (24850-33-7;105494-65-3;66680-84-0;66680-85-1)
SOL 6 (75-05-8), MeCN
CAT 1250 (16774-21-3), (NH₄)₂Ce(NO₃)₆
PRO III, 868577
YDS 90.0 %
T 25.0 Cel
TIM 0.3 - 0.7 hr
KW addition; alkylation; C-alkylation
NTE reaction:I (II) -> III, example: 7

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Amberlyst-15[®] as a Novel and Recyclable Solid Acid for the Coupling of

10/500,718

Aromatic Aldehydes with Homopropargyl Alcohol.

RX(4) OF 6 A + J ==> K



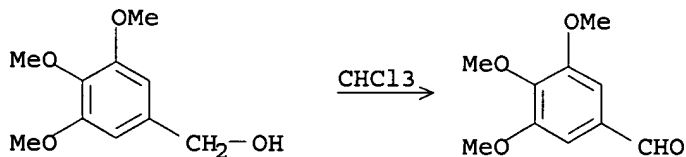
III
YIELD 72.0%

RX(4) RCT I, 20574 (927-74-2)
 II, 43670 (86-81-7)
 SOL 60 (75-09-2), CH2Cl2
 CAT 5247 (9037-24-5), Amberlyst 15
 PRO III, 1082110
 YDS 72.0 %
 T 25.0 Cel
 KW olefination; alkylation; O-alkylation; etherification
 NTE reaction: I (II) -> III, example: 4

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Oxidation of alcohols with tetra-n-butylammonium chromate

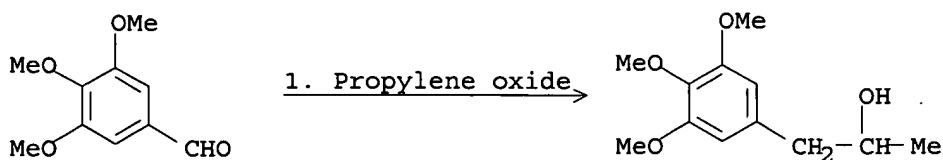
RX(1) OF 13



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Antiulcer formulation containing deoxyschizandrin

RX(5) OF 7 - 2 STEPS

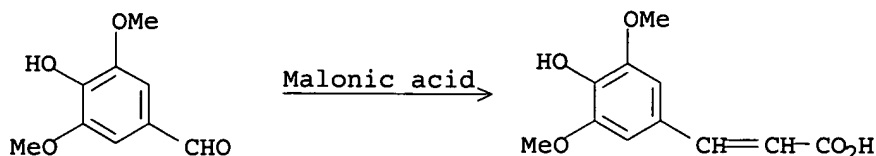


10/500,718

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis of sinapyl alcohol diisovalerate, a new phenylpropanoid from *Artemisia ASSOANA*

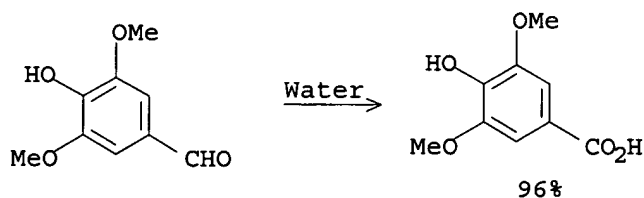
RX(1) OF 15



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Continuous oxidation of aromatic aldehyde to aromatic carboxylic acid by *Burkholderia cepacia* TM1 in a cell-holding reactor

RX(3) OF 3

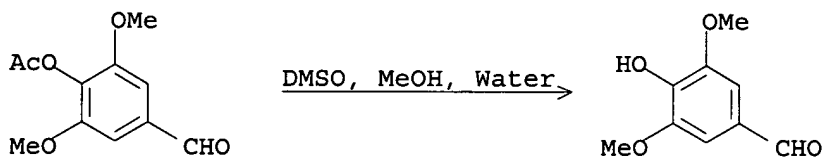


NOTE: biotransformation, buffered soln., cell-holding reactor, oxidn. by *Burkholderia cepacia* TM1

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Rigid-rod β -barrel ion channels with internal "Cascade Blue" cofactors - catalysis of amide, carbonate, and ester hydrolysis

RX(20) OF 43

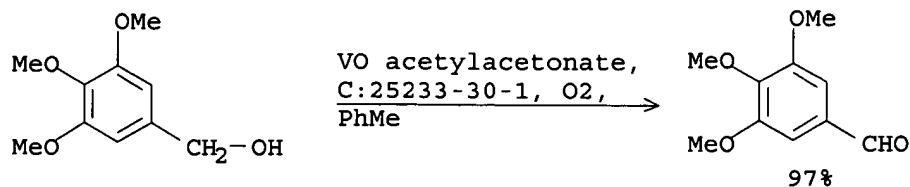


NOTE: buffered soln.

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Polyaniline supported vanadium catalyzed aerobic oxidation of alcohols to aldehydes and ketones

RX(4) OF 13



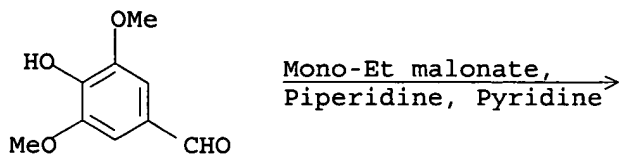
NOTE: solid-supported catalyst

10/500,718

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI First total synthesis of (±)-Aiphanol

RX(1) OF 64

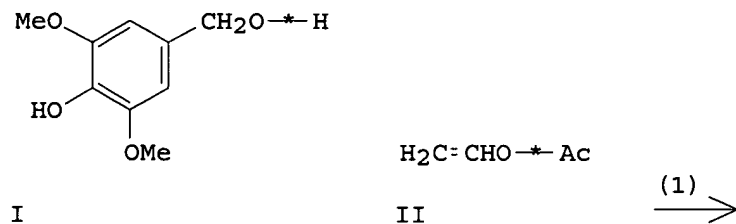


NOTE: stereoselective

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Lipase-Catalyzed Chemoselective Monoacetylation of Hydroxyalkylphenols and Chemoselective Removal of a Single Acetyl Group from Their Diacetates.

RX(1) OF 22 A + B ==> C



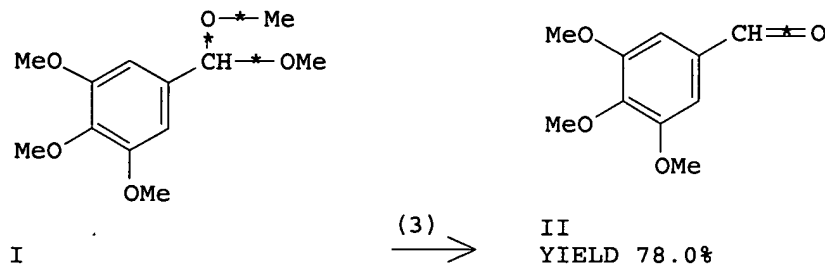
RX(1) RCT I, 23771 (530-56-3)
II, 2703 (108-05-4)
RGT 6203 (9001-62-1), triacylglycerol lipase
SOL 250 (108-20-3), iPr2O
PRO III, 650174
YDS 98.0 %
T 25.0 Cel
KW acetylation; acylation; O-acylation; esterification
NTE reaction:I (II) -> III, example: 1

10/500,718

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Highly Efficient Deprotection of Aromatic Acetals under Neutral Conditions Using β -Cyclodextrin in Water.

RX(3) OF 8 G ==> H

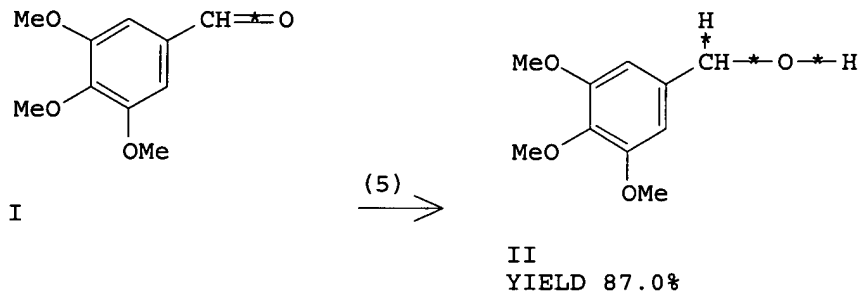


RX(3) RCT I, 77950 (59276-37-8)
SOL 222 (7732-18-5), H₂O
CAT 2514 (7585-39-9;130322-66-6;130322-68-8), CHIRAL, beta-cyclodextrin
PRO II, 43670 (86-81-7)
YDS 78.0 %
T 50.0 Cel
NTE reaction:I -> II, example: 4

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Selective Reduction of Aldehydes to Alcohols Using Alumina with a Catalytic Amount of Base under Microwave Irradiation.

RX(5) OF 5 L ==> M



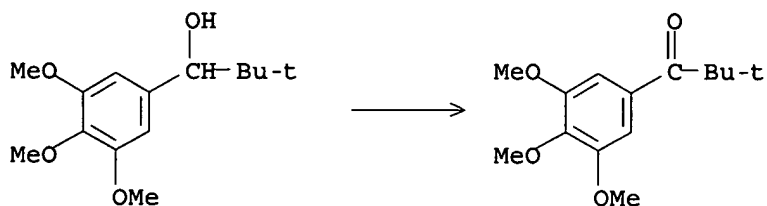
RX(5) RCT I, 43670 (86-81-7)
SOL 123 (67-56-1), MeOH
CAT 1134 (1122-58-3), DMAP
11 (1344-28-1;1302-74-5;1317-82-4;12174-49-1), Al₂O₃
PRO II, 203015 (3840-31-1)
YDS 87.0 %
TIM 0.1 - 0.2 hr
KW addition; hydrogenation
NTE reaction:I -> II, example: 5

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Preparation and NMR spectra of 2,5-diaryl-2,5-di-tert-butyl- Δ^3 -1,3,4-thiadiazoline 1,1-dioxides

10/500,718

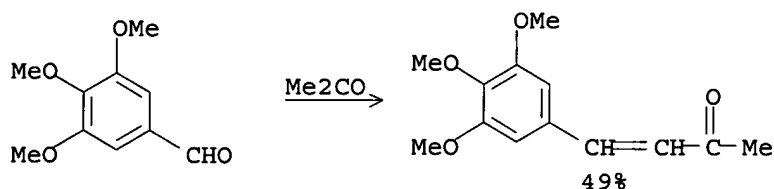
RX(1) OF 4



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Antiepileptic and antileukemic thiosemicarbazones and semicarbazones of 4-aryl-3-buten-2-ones

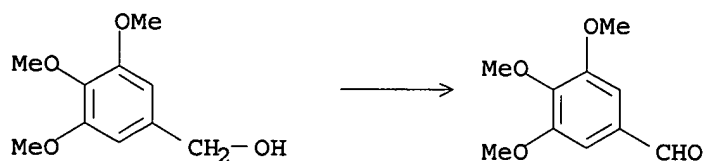
RX(18) OF 36



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Syntheses of 5,3',4',5'-tetramethoxy-6,7-methylenedioxyisoflavone and 5,3',4'-trimethoxy-6,7-methylenedioxyisoflavone isolated from *Iris germanica* rhizomes

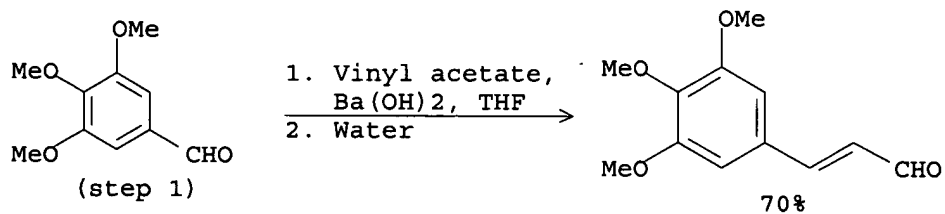
RX(1) OF 65



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Formation of acetaldehyde enolate from vinyl acetate and its reaction with aromatic and heterocyclic aldehydes: an efficient synthesis of enals and polyenals

RX(9) OF 38



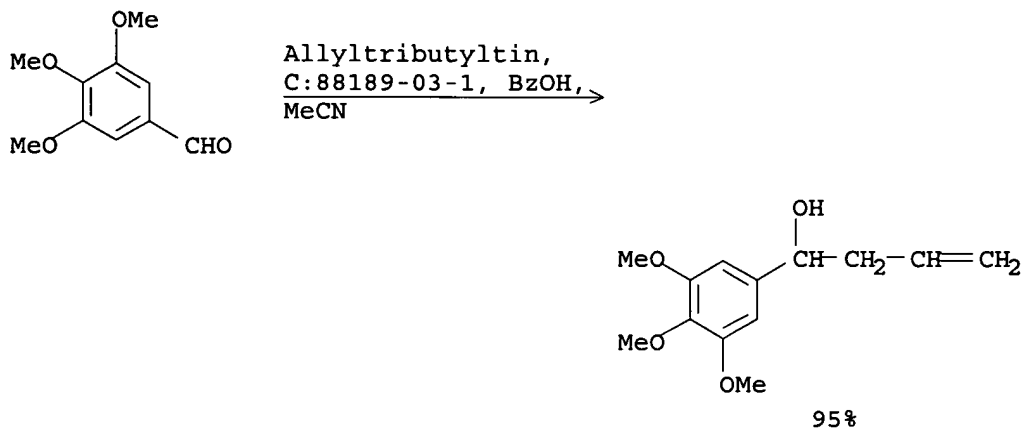
NOTE: stereoselective

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

10/500,718

TI Highly efficient allylation of aldehydes and three-component synthesis of homoallylamines using bismuth triflate catalyst

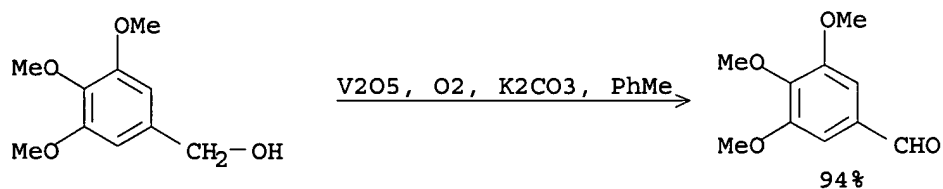
RX(4) OF 20



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Novel Vanadium-Catalyzed Oxidation of Alcohols to Aldehydes and Ketones under Atmospheric Oxygen

RX(4) OF 16

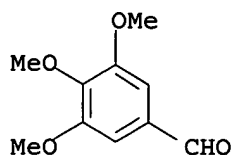


L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

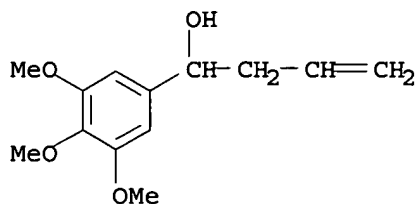
TI Microencapsulated bismuth(III) triflate catalyst for organic transformations

10/500,718

RX(1) OF 28



Allyltributyltin,
C:88189-03-1, BzOH,
MeCN

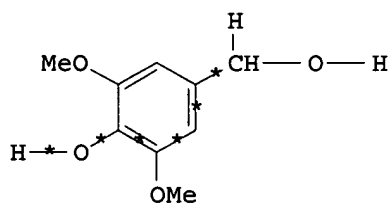


95%

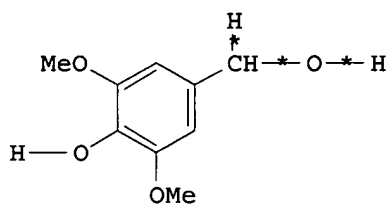
NOTE: solid-supported catalyst on polystyrene, microencapsulated catalyst is reusable, green chem.-catalyst

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Cobalt-Schiff Base Complex Catalyzed Oxidation of para-Substituted Phenolics. Preparation of Benzoquinones.

RX(1) OF 6 2 A ==> B + C...

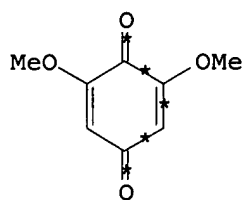


I

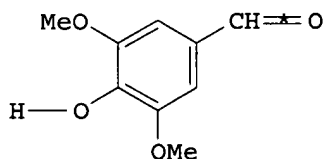


I

(1) >



II
YIELD 88.0%

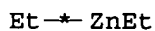
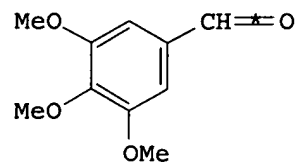


III
YIELD 4.0%

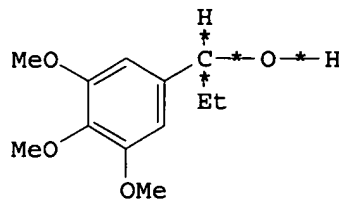
RX(1) RCT I, 23771 (530-56-3)
RGT 157 (7782-44-7), O2
SOL 123 (67-56-1), MeOH
CAT 401237, Co(py)(salen)
PRO II, 132665 (530-55-2)
III, 178409 (134-96-3)
YDS 92.0 %
KW dearomatisation; dehydrogenation
NTE reaction: I -> II + III, example: 1
CMT Ratio = 1:2 for products 1,2

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
 TI New Polymer Anchored Chiral Amino Oxazolines as Effective Catalysts for
 Enantioselective Addition of Diethylzinc to Aldehydes.

RX(6) OF 6 O + B ==> P



(6) \longrightarrow

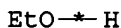
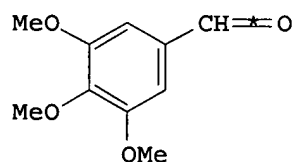


YIELD 86.0%

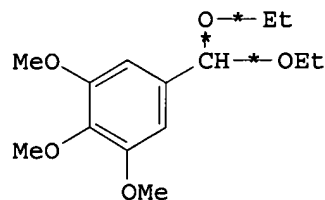
RX(6) RCT II, 43670 (86-81-7)
 III, 970 (557-20-0)
 SOL 214 (108-88-3), toluene
 60 (75-09-2), CH₂Cl₂
 CAT 905918, CHIRAL, (S,S)-4-sBu-2-(2-(NH-CH₂-polystyrene)-C₆H₄)-2-oxazoline
 PRO IV, 910332, (R)-isomer
 YDS 86.0 %
 T 0.0 Cel
 TIM 24 hr
 EEXP 1 90.0 %
 KW addition; alkylation; C-alkylation
 NTE reaction:II (III) -> (R)-IV, example: 6

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
 TI Cobalt(II)-Catalyzed Chemoselective Synthesis of Acetals from Aldehydes.

RX(6) OF 11 N + J ==> O



(6) \longrightarrow



YIELD 67.0%

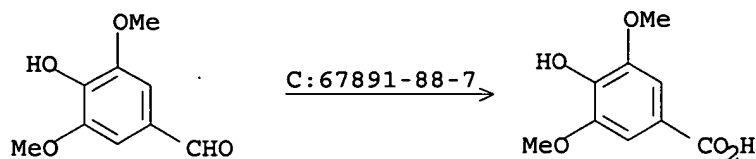
RX(6) RCT I, 43670 (86-81-7)
 II, 81 (64-17-5)
 CAT 330 (7646-79-9), CoCl₂
 PRO III, 77952 (101403-71-8)
 YDS 67.0 %
 T.KW REFLUX
 KW alkylation; O-alkylation; etherification
 NTE reaction:I (II) -> III, example: 6

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI The metabolism of aromatic compounds related to lignin by some
 hyphomycetes and yeastlike fungi of soil

10/500,718

RX(27) OF 31

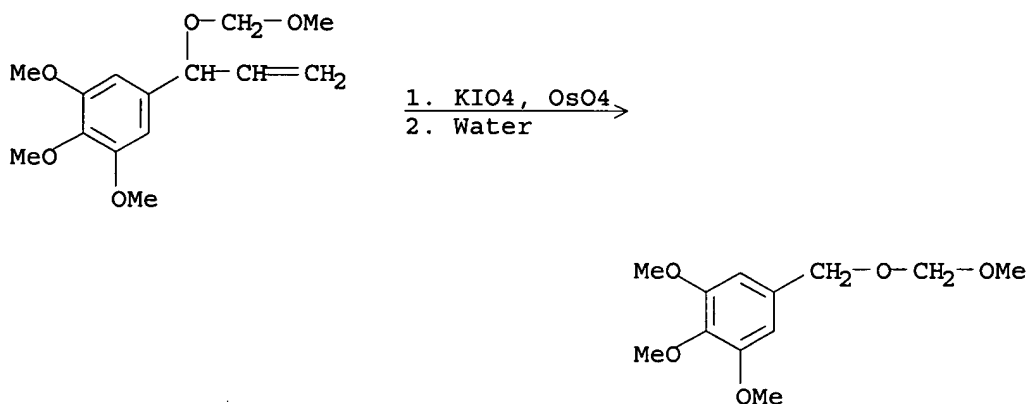


NOTE: Biotransformation: catalyzed by pullularia pullulans; #
Conditions: study on metabolism and degradation

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI An efficient procedure for the mild oxidative cleavage of alkene-3-ols:
application to the preparation of 2-alkoxy-2-(3,4,5-trimethoxyphenyl)acetaldehyde

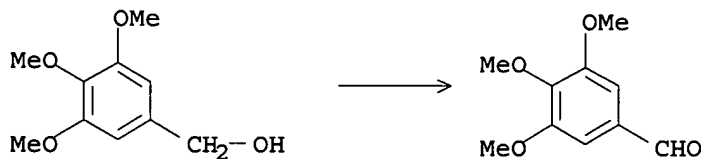
RX(15) OF 21 - 2 STEPS



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Oxidation of methoxylated benzyl alcohols by laccase of Coriolus
versicolor in the presence of syringaldehyde

RX(2) OF 4

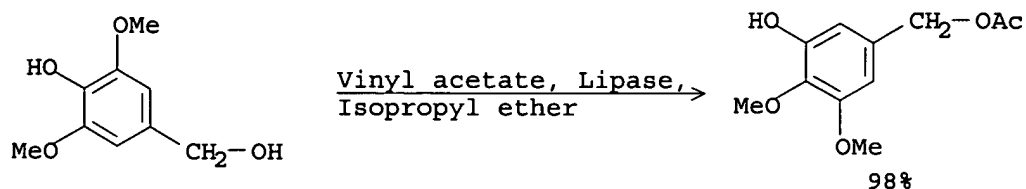


L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Lipase-catalyzed chemoselective monoacetylation of hydroxyalkylphenols and
chemoselective removal of a single acetyl group from their diacetates

10/500,718

RX(1) OF 35

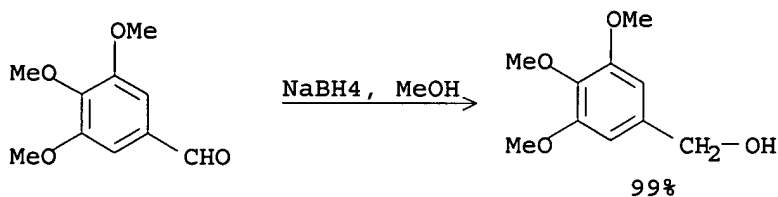


NOTE: STEREOSELECTIVE, ENZYMIC

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis and biological activity of isoamoenylin, a metabolite of *Dendrobium amoenum*

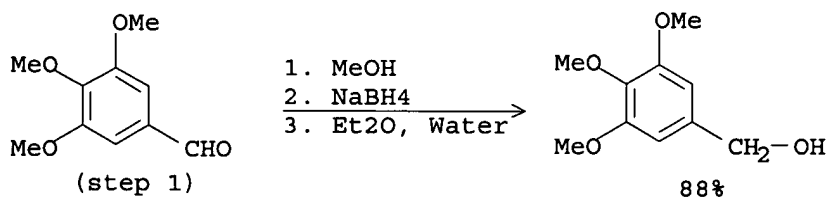
RX(1) OF 17



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Regioselective reductive demethoxylation of 3,4,5-trimethoxystilbenes

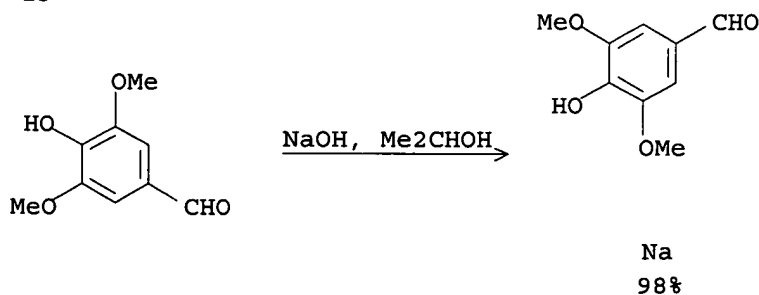
RX(1) OF 78



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis of 4-(4'-formylaryloxy)-7-nitrobenzofurazan derivatives from 4-chloro-7-nitrobenzofurazan and some formylphenols in the presence of crown ethers

RX(4) OF 15

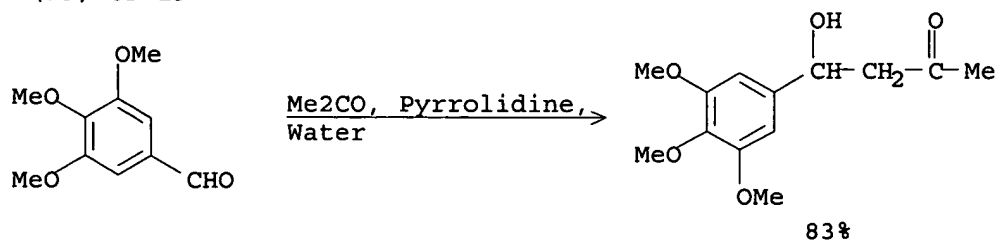


L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

10/500,718

TI Electron deficiency of aldehydes controls the pyrrolidine catalyzed direct cross-aldol reaction of aromatic/heterocyclic aldehydes and ketones in water

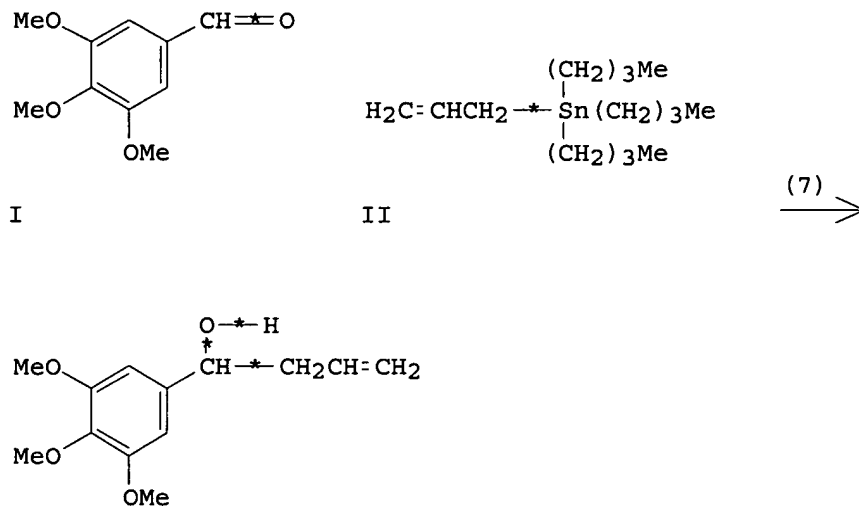
RX(19) OF 19



L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Lanthanum Triflate Catalyzed Allylation of Aldehydes: Crucial Activation by Benzoic Acid.

RX(7) OF 7 Q + B ==> R



III
YIELD 88.0%

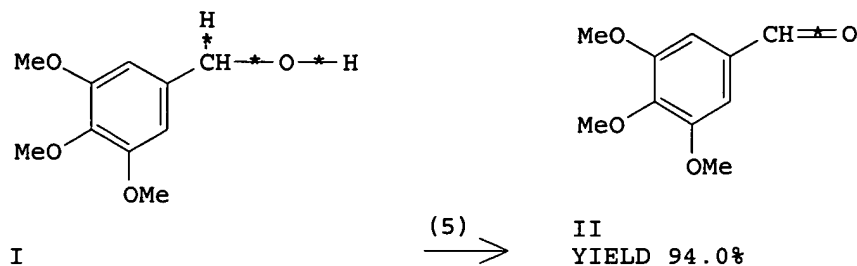
RX(7) RCT I, 43670 (86-81-7)
II, 1987 (24850-33-7;105494-65-3;66680-84-0;66680-85-1)
RGT 475 (65-85-0), Ph-COOH
SOL 6 (75-05-8), MeCN
CAT 393196, La(OTf)₃
PRO III, 868577
YDS 88.0 %
T 25.0 Cel
KW addition; alkylation; C-alkylation
NTE reaction:I (II) -> III, example: 7

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Novel Vanadium-Catalyzed Oxidation of Alcohols to Aldehydes and Ketones under Atmospheric Oxygen.

RX(5) OF 12 M ==> N

10/500,718

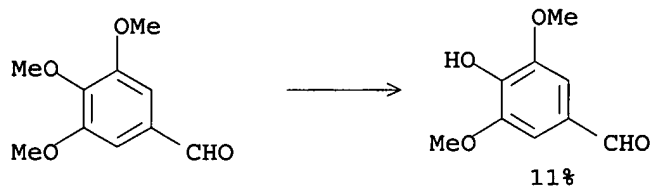


RX(5) RCT I, 203015 (3840-31-1)
RGT 768 (584-08-7), K2CO3
157 (7782-44-7), O2
SOL 214 (108-88-3), toluene
CAT 1263 (1314-62-1), V2O5
PRO II, 43670 (86-81-7)
YDS 94.0 %
T 100.0 Cel
TIM 24 hr
KW dehydrogenation
NTE reaction:I -> II, example: 5

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI The alkaline nitrobenzene oxidation of aspen wood and lignin model substances

RX(1) OF 1

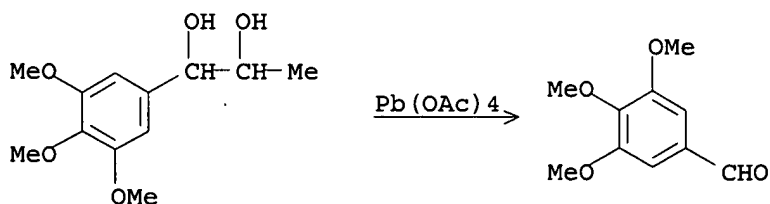


NOTE: Classification: Hydrolysis; Hydroxylation; Nucleophilic substitution; # Conditions: NaOH; PhNO2; # Comments: also Chem Abs, 8597c (1955)

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A synthesis of 5,6,7-trimethoxyisocoumarin-3-carboxylic acid and related studies

RX(2) OF 29

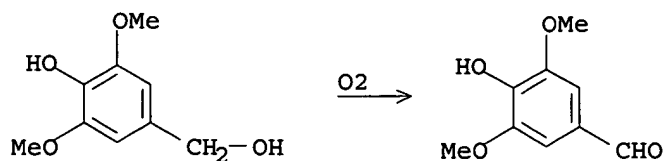


L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Bisabolones and other constituents of Mikania shushunensis

10/500,718

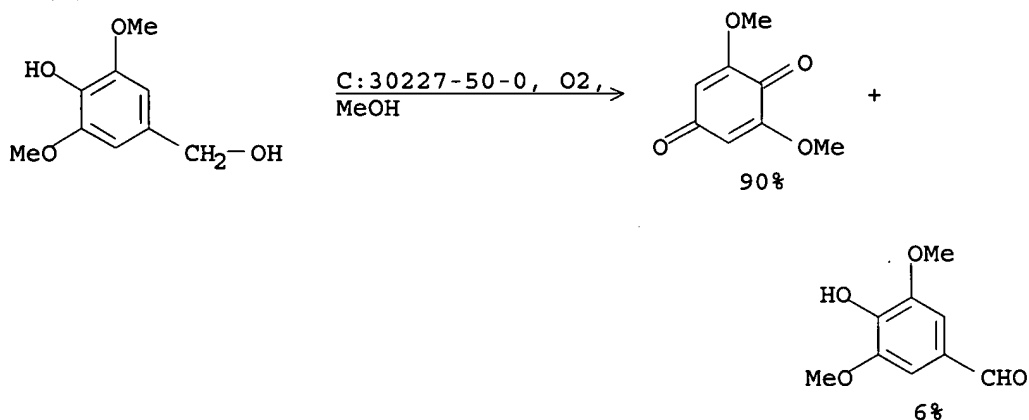
RX(1) OF 2



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Cobalt-Schiff Base Complex Catalyzed Oxidation of Para-Substituted Phenolics. Preparation of Benzoquinones

RX(1) OF 9

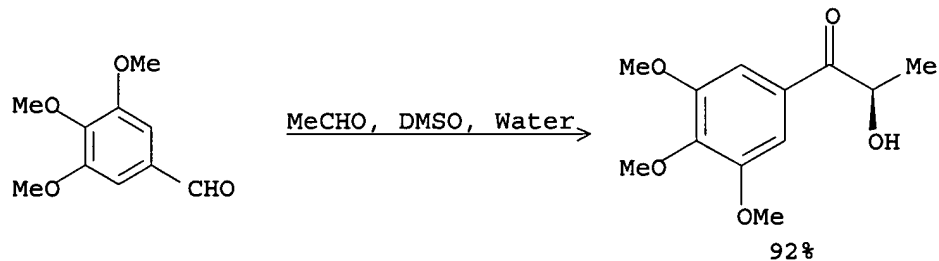


NOTE: PRODUCT DISTRIBUTION AFFECTED BY CATALYST

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Enantioselective synthesis of α -hydroxy ketones via benzaldehyde lyase-catalyzed C-C bond formation reaction

RX(34) OF 35



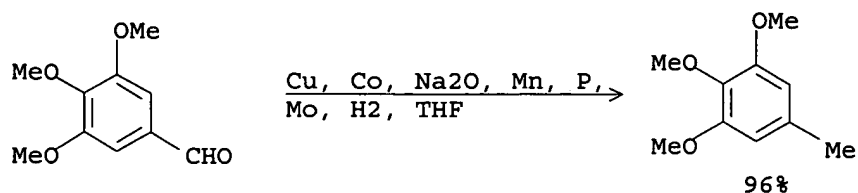
NOTE: biotransformation, biocatalyst used, Benzaldehyde lyase from *Pseudomonas fluorescens* Biovar I used, potassium phosphate buffered soln., pH 7.0, stereoselective

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Hydrogenolysis process and catalysts for producing 3,4,5-trisubstituted toluene derivatives from their corresponding benzyl alcohols or benzaldehydes

10/500,718

RX(1) OF 1

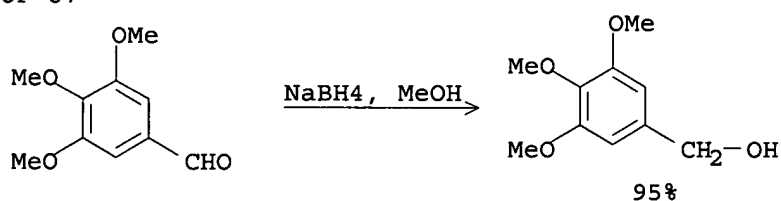


NOTE: high pressure, other catalysts gave similar yields

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI A new family of quinoline and quinoxaline analogues of combretastatins

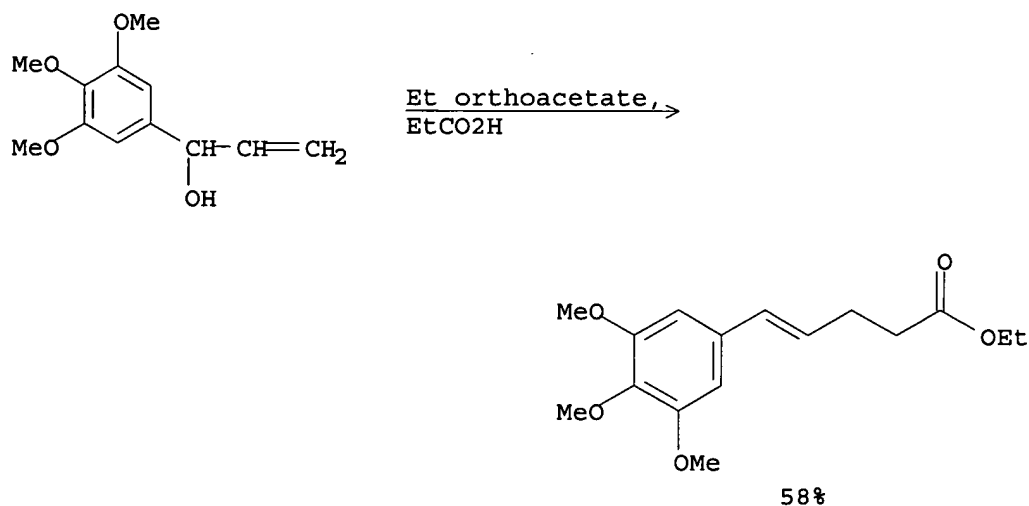
RX(21) OF 87



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis and biological activity of the tea catechin metabolites, M4 and M6 and their methoxy-derivatives

RX(11) OF 75



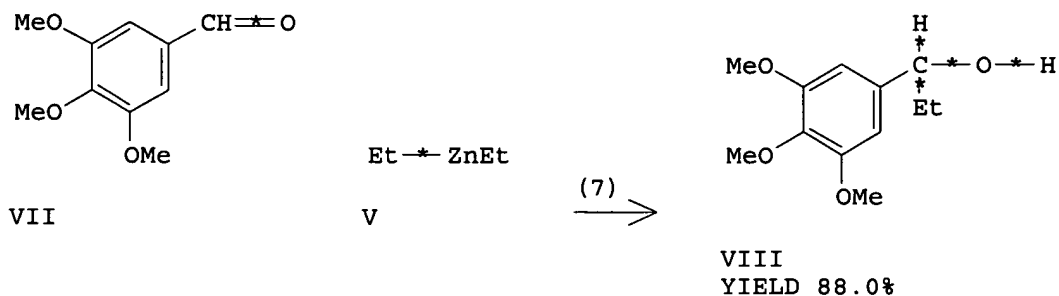
NOTE: stereoselective, Claisen reaction

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI A Practical o-Hydroxybenzylamine-Promoted Enantioselective Addition of Dialkylzincs to Aldehydes with Asymmetric Amplification.

RX(7) OF 12 P + B ==> Q

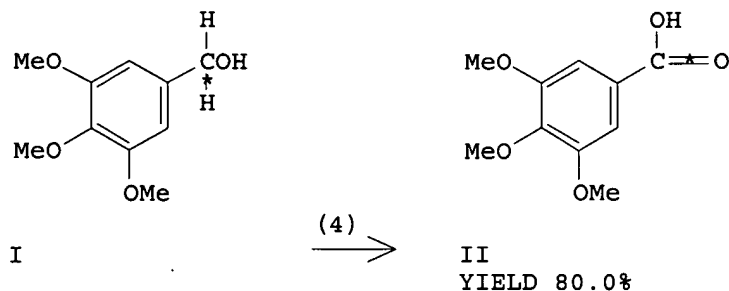
10/500,718



RX(7) RCT VII, 43670 (86-81-7)
 V, 970 (557-20-0)
 SOL 214 (108-88-3), toluene
 CAT 679529, CHIRAL, (2-OH-C6H4) - (R) - CHPh-NH- (R) - CHMe-Ph
 PRO VIII, 790694, (S)-isomer
 YDS 88.0 %
 T 25.0 Cel
 TIM 5.0 hr
 EEXP 1 86.0 %
 KW addition; alkylation; C-alkylation
 NTE reaction:VII (V) -> (S)-VIII, example: 2

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
 TI Cobalt(II)-Catalyzed Oxidation of Alcohols into Carboxylic Acids and Ketones with Hydrogen Peroxide.

RX(4) OF 8 K ==> L



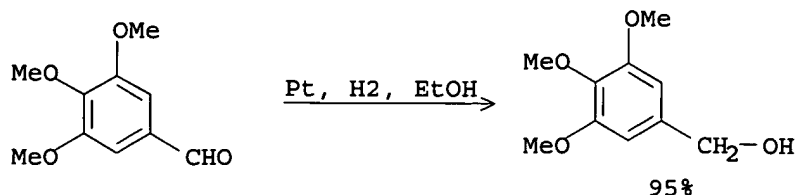
RX(4) RCT I, 203015 (3840-31-1)
 RGT 1158 (7722-84-1), H2O2
 157 (7782-44-7), O2
 SOL 6 (75-05-8), MeCN
 CAT 974203, Co(H4-salen)
 PRO II, 14547 (118-41-2)
 YDS 80.0 %
 T 80.0 Cel
 TIM 4.0 hr
 NTE reaction:I -> II, example: 4

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Colchicine and related compounds. III

10/500,718

RX(1) OF 1

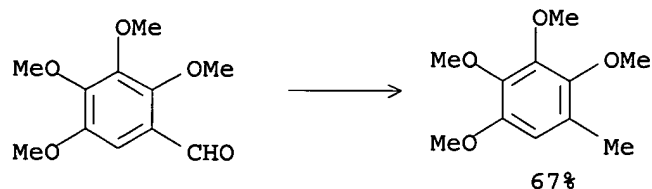


NOTE: Classification: Hydrogenation; Chemoselective; # Conditions: Pt-C/H₂ EtOH 15h

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis of ubiquinone and menaquinone analogs by oxidative demethylation of alkenylhydroquinone ethers with argentic oxide or ceric ammonium nitrate in the presence of 2,4,6-pyridinetricarboxylic acid

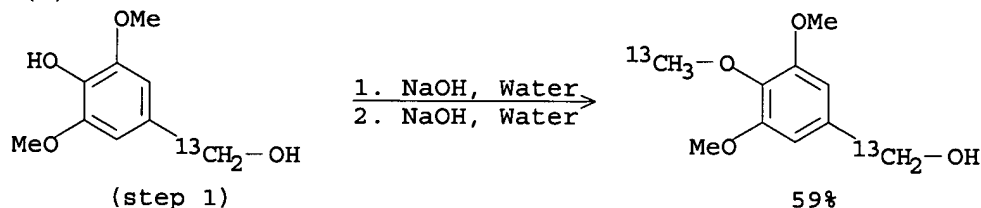
RX(15) OF 95



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Selectively carbon-13 enriched 2,4-diamino-5-(3,4,5-trimethoxybenzyl)pyrimidine (Trimethoprim) and 2,4-diaminopyrimidine

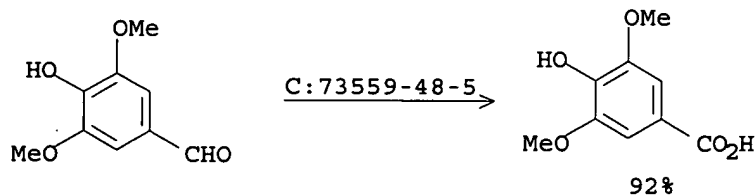
RX(2) OF 64



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Oxidation of aromatic aldehydes by *Serratia marcescens*

RX(8) OF 13



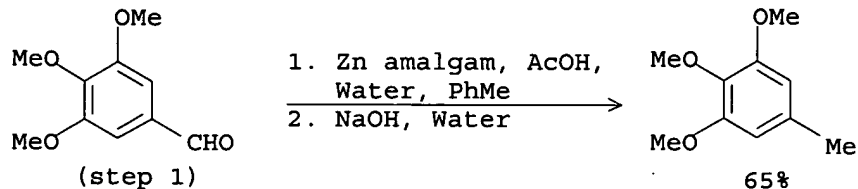
NOTE: Biotransformation: catalyzed by *serratia marcescens*; # Conditions: 0,3% (w/v) educt; resuspended cells, from 200 ml culture, grown with vanillin; 100 ml p-buffer ph 7,0; 230 h, 28.deg.c

10/500,718

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Synthesis of 2,3-dimethoxy-5-methyl-1,4-benzoquinone: a key fragment in coenzyme-Q series

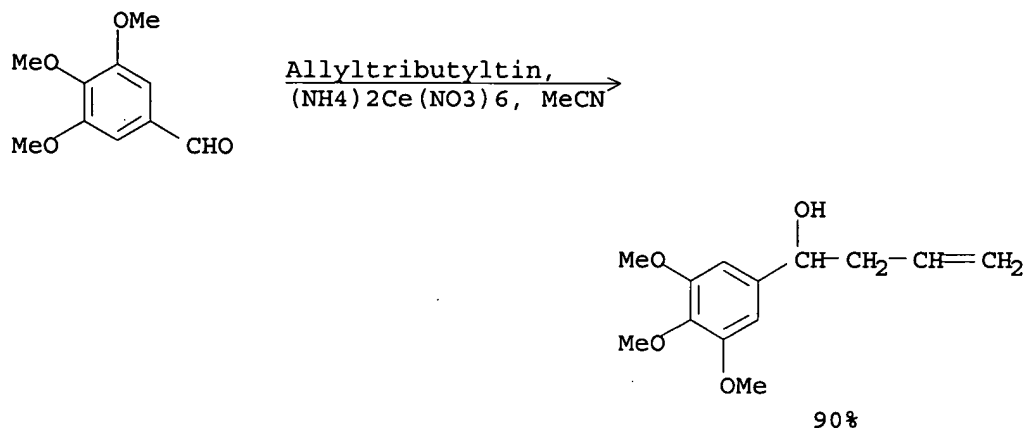
RX(4) OF 15



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Ceric(IV) ammonium nitrate: A novel reagent for the synthesis of homoallyl alcohols

RX(3) OF 26

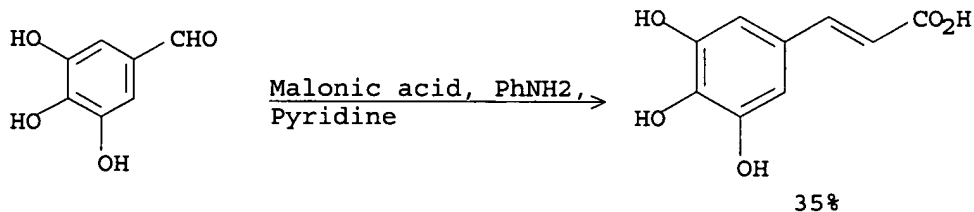


NOTE: chemoselective

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Conformational analysis of a trihydroxylated derivative of cinnamic acid-a combined Raman spectroscopy and ab initio study

RX(1) OF 2



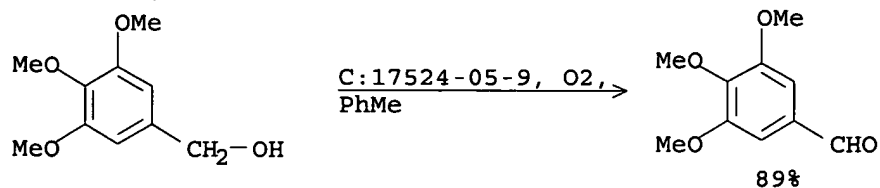
NOTE: stereoselective

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Novel Polyaniline-Supported Molybdenum-Catalyzed Aerobic Oxidation of Alcohols to Aldehydes and Ketones

10/500,718

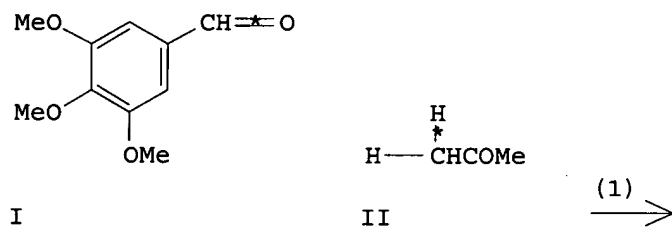
RX(5) OF 17



NOTE: solid-supported catalyst, polyaniline supported molybdenum, green chem. - catalyst

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Open Analogues of Arcyriaflavin A. Synthesis Through Diels-Alder Reaction between Maleimides and 1-Aryl-3-tert-butyldimethylsiloxy-1,3-butadienes.

RX(1) OF 111 A + B ==> C...



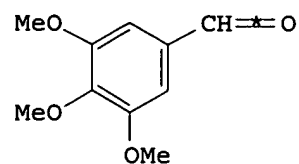
III
YIELD 78.0%

RX(1) RCT I, 43670 (86-81-7)
II, 5 (67-64-1)
RGT 1159 (1310-73-2), NaOH
SOL 81 (64-17-5), EtOH
222 (7732-18-5), H₂O
PRO III, 763927
YDS 78.0 %
KW olefination
NTE reaction: I (II) -> III, example: 1

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
TI Enhanced Effect of Mesoporous Silica on Base-Catalyzed Aldol Reaction.

RX(8) OF 8 2 Q + 2 B ==> R + S

10/500,718



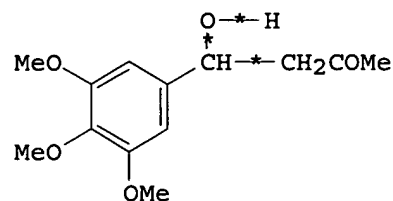
2 V



II

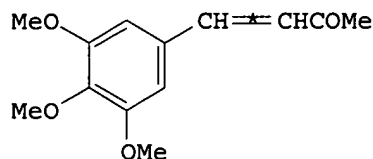


II



VI

YIELD 17.0%



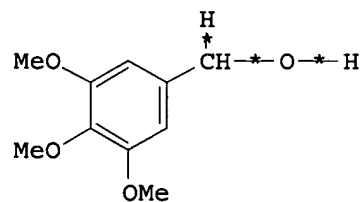
VII

YIELD 19.0%

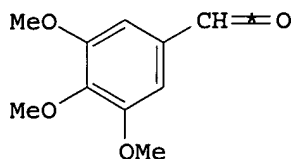
RX(8) RCT V, 43670 (86-81-7)
 II, 5 (67-64-1)
 CAT 180 (110-89-4), piperidine
 192 (7631-86-9), SiO₂
 PRO VI, 644681
 VII, 763927
 YDS 36.0 %
 T 30.0 Cel
 KW addition; alkylation; C-alkylation; olefination
 NTE reaction: V (II) -> VI + VII, example: 4

L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN
 TI Novel Polyaniline-Supported Molybdenum-Catalyzed Aerobic Oxidation of
 Alcohols to Aldehydes and Ketones.

RX(3) OF 14 H ==> I



I



II
 YIELD 89.0%



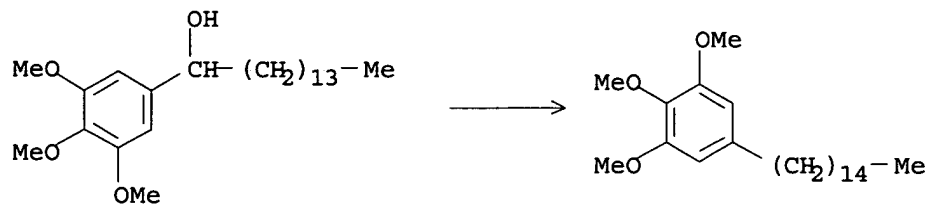
RX(3) RCT I, 203015 (3840-31-1)
 RGT 157 (7782-44-7), O₂
 SOL 214 (108-88-3), toluene
 CAT 1071051, MoO₂(acac)₂(polyaniline)
 PRO II, 43670 (86-81-7)
 YDS 89.0 %
 T 100.0 Cel
 KW dehydrogenation
 NTE reaction: I -> II, example: 3

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

10/500,718

TI Side reactions in hydrogenolyses of substituted benzylic alcohols with palladium-carbon catalysts

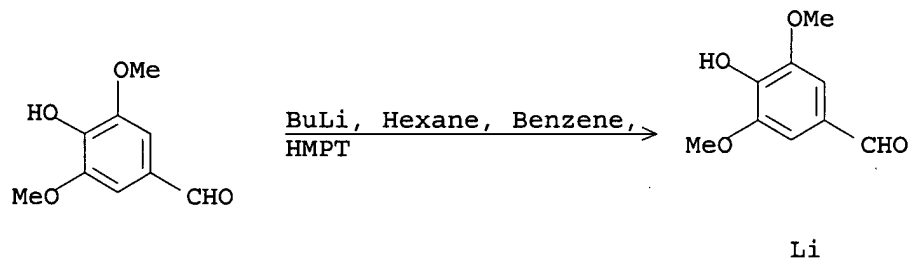
RX(4) OF 7



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Total synthesis and study of biologically active lignans. 8. Total synthesis of 5-methoxyisolariciresinol

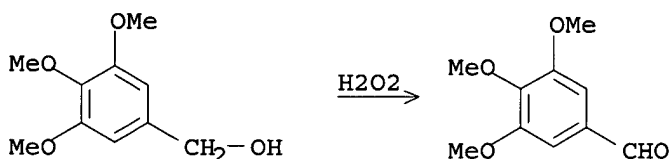
RX(9) OF 144



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Enzyme-catalyzed oxidation of non-phenolic aromatic compounds

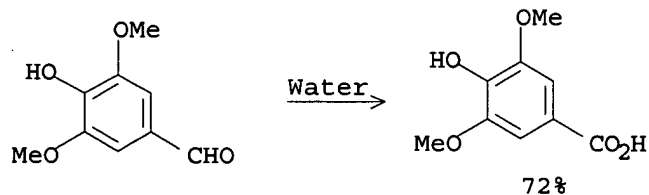
RX(4) OF 6



L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Oxidation of aromatic aldehyde to aromatic carboxylic acid by Burkholderia cepacia TM1 isolated from humus

RX(3) OF 3



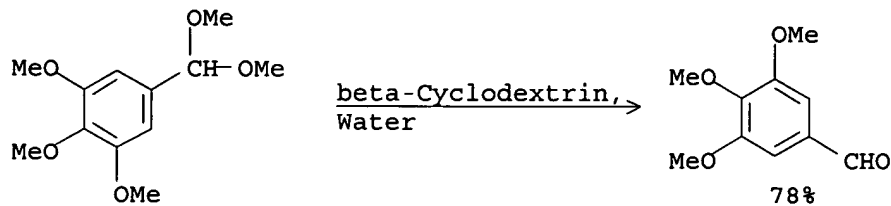
NOTE: BIOTRANSFORMATION

10/500,718

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Highly Efficient Deprotection of Aromatic Acetals under Neutral Conditions Using β -Cyclodextrin in Water

RX(9) OF 15

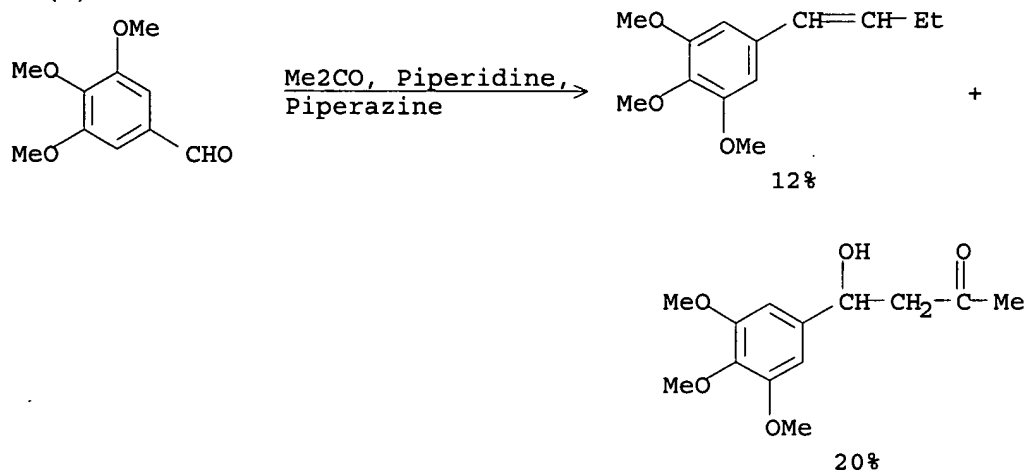


NOTE: green chem. - solvent

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Method for synthesis of β -hydroxy ketone by Claisen-Schmidt reaction of aromatic aldehydes with ketones and catalysts therefor

RX(2) OF 2

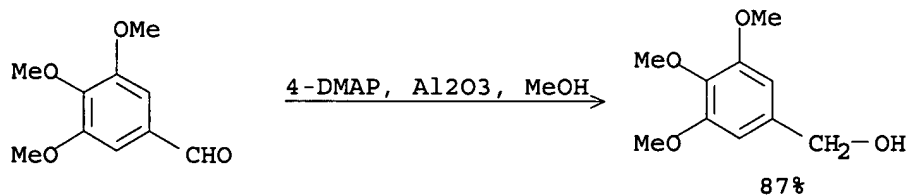


NOTE: Claisen-Schmidt reaction (addn. reaction)

L13 92 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Selective reduction of aldehydes to alcohols using alumina with a catalytic amount of base under microwave irradiation

RX(9) OF 14



NOTE: microwave irradiation

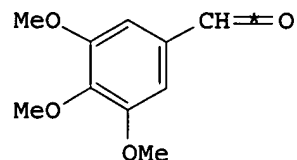
L13 92 ANSWERS CHEMINFORMRX COPYRIGHT 2006 FIZ CHEMIE on STN

TI Aldol and Knoevenagel Condensations Catalyzed by Modified Mg-Al

10/500,718

Hydrotalcite: A Solid Base as Catalyst Useful in Synthetic Organic Chemistry.

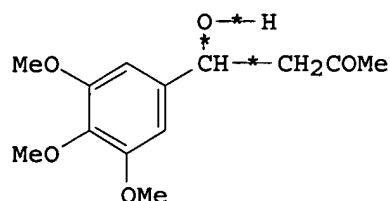
RX(2) OF 12 F + B ==> G



I



II



III

YIELD 98.0%

RX(2) RCT I, 43670 (86-81-7)
II, 5 (67-64-1)
SOL 5102, neat
CAT 401112 (12304-65-3), hydrotalcite
PRO III, 644681
YDS 98.0 %
T 25.0 Cel
KW addition; alkylation; C-alkylation
NTE reaction:I (II) -> III, example: 2

ALL ANSWERS HAVE BEEN SCANNED

=> file stnguide

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

3.11

829.64

FILE 'STNGUIDE' ENTERED AT 10:03:21 ON 29 APR 2006

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 21, 2006 (20060421/UP).

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.02

830.66

FILE 'CASREACT' ENTERED AT 10:13:32 ON 29 APR 2006

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FILE CONTENT:1840 - 23 Apr 2006 VOL 144 ISS 17

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 10 million reactions   *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 09:38:34 ON 29 APR 2006)

FILE 'REGISTRY' ENTERED AT 09:38:39 ON 29 APR 2006

L1 STRUCTURE UPLOADED
L2 QUE L1

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:39:12 ON 29 APR 2006

L3 36 S L2

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:43:11 ON 29 APR 2006

L4 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L5 STRUCTURE UPLOADED
L6 QUE L5 NOT L4

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:43:37 ON 29 APR 2006

L7 8 S L6
L8 92 S L6

FILE 'STNGUIDE' ENTERED AT 09:45:49 ON 29 APR 2006

FILE 'REGISTRY' ENTERED AT 09:47:47 ON 29 APR 2006

L9 SCREEN 1992 OR 2009 OR 2016 OR 2021 OR 2026 OR 1929 OR 18
L10 STRUCTURE UPLOADED
L11 QUE L10 NOT L9

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:48:18 ON 29 APR 2006

L12 8 S L11
L13 92 S L11

FILE 'STNGUIDE' ENTERED AT 09:59:16 ON 29 APR 2006

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 09:59:56 ON 29 APR 2006

10/500,718

FILE 'STNGUIDE' ENTERED AT 10:00:28 ON 29 APR 2006

FILE 'CASREACT, CHEMINFORMRX, DJSMONLINE, PS' ENTERED AT 10:01:51 ON 29 APR 2006

FILE 'STNGUIDE' ENTERED AT 10:03:21 ON 29 APR 2006

FILE 'CASREACT' ENTERED AT 10:13:32 ON 29 APR 2006

=> s l13 and cu?

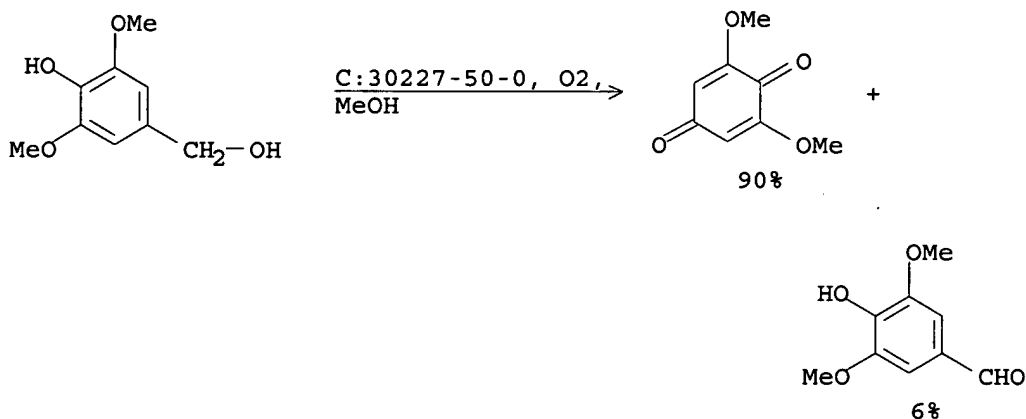
37179 CU?

L14 5 L13 AND CU?

=> d 1-5

L14 ANSWER 1 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 9

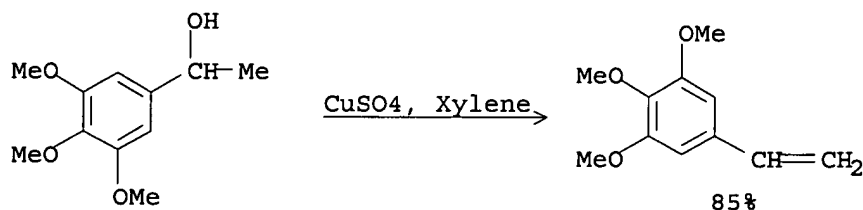


REF: Journal of Organic Chemistry, 60(8), 2398-404; 1995

NOTE: PRODUCT DISTRIBUTION AFFECTED BY CATALYST

L14 ANSWER 2 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 3



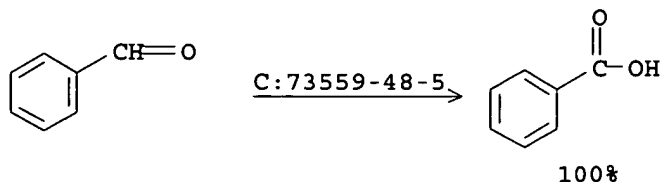
REF: Czech., 276700, 15 Jul 1992

NOTE: reflux, removal of H2O, 3 h

L14 ANSWER 3 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

10/500,718

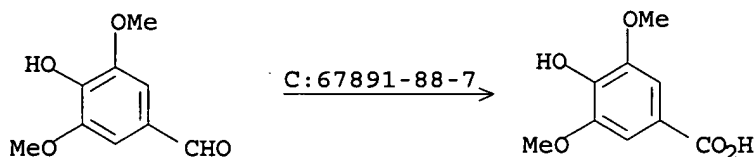
RX(1) OF 13



REF: Applied and Environmental Microbiology, 57(4), 1275-6; 1991
NOTE: Biotransformation: catalyzed by *serratia marcescens*; #
Conditions: 0,2% (w/v) educt; resuspended cells, from 200 ml culture, grown with vanillin; 100 ml p-buffer ph 7,0; 45 h, 28.deg.c

L14 ANSWER 4 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

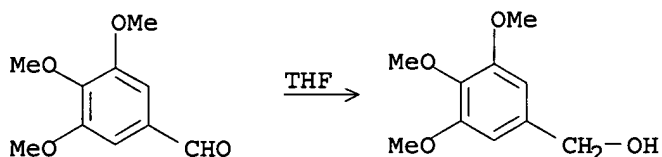
RX(27) OF 31



REF: Journal of General Microbiology, 26,, 155-65; 1961
NOTE: Biotransformation: catalyzed by *pullularia pullulans*; #
Conditions: study on metabolism and degradation

L14 ANSWER 5 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(2) OF 11



REF: Journal of the American Chemical Society, 81,, 2805-13; 1959
NOTE: Classification: Reduction; # Conditions: LiAlH₄ THF Rf 5h

=> s l13 methyl-substituted or 3,4,5-trisubstituted toluene

MISSING OPERATOR L13 METHYL-SUBS

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l13 and (methyl-substituted or 3,4,5-trisubstituted toluene)

117945 METHYL
84663 SUBSTITUTED
708 METHYL-SUBSTITUTED
(METHYL(W) SUBSTITUTED)
333049 3
315473 4
243530 5
2819 TRISUBSTITUTED
15778 TOLUENE
1 3,4,5-TRISUBSTITUTED TOLUENE

10/500,718

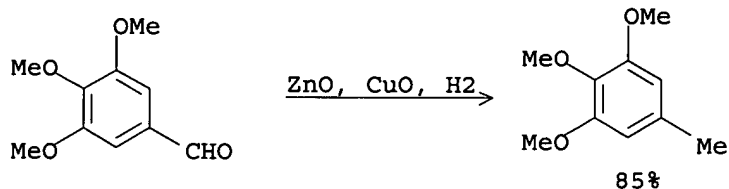
(3 (W) 4 (W) 5 (W) TRISUBSTITUTED (W) TOLUENE)

L15 2 L13 AND (METHYL-SUBSTITUTED OR 3,4,5-TRISUBSTITUTED TOLUENE)

=> d 1-2

L15 ANSWER 1 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 10



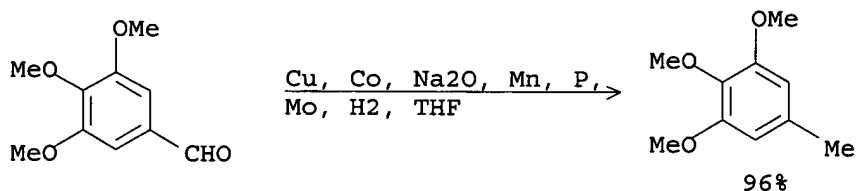
REF: PCT Int. Appl., 2003095399, 20 Nov 2003

NOTE: thermal

CON: 10 hours, 230 deg C, 5 MPa

L15 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 1



REF: PCT Int. Appl., 2003062174, 31 Jul 2003

NOTE: high pressure, other catalysts gave similar yields

CON: 180 deg C, 200 bar

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

38.23

868.89

STN INTERNATIONAL LOGOFF AT 10:18:45 ON 29 APR 2006